WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 01:44 AM EDT

PDB ID	:	3OTR
Title	:	2.75 Angstrom Crystal Structure of Enolase 1 from Toxoplasma gondii
Authors	:	Minasov, G.; Ruan, J.; Shuvalova, L.; Halavaty, A.; Ngo, H.; Tomavo, S.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2010-09-13
Resolution	:	2.75 Å(reported)

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

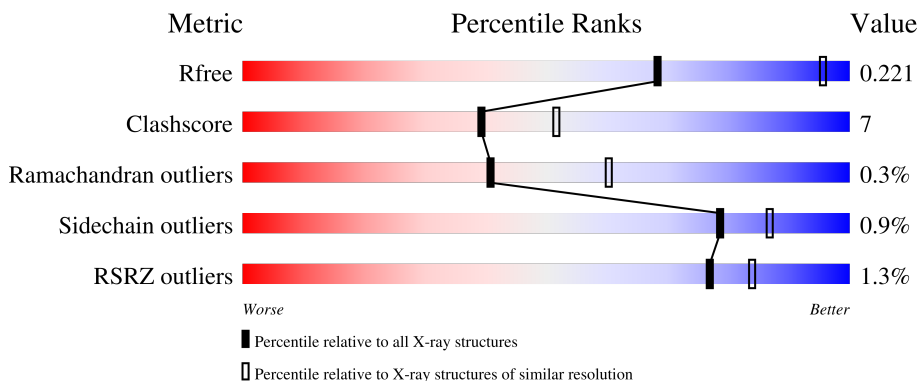|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.75 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.
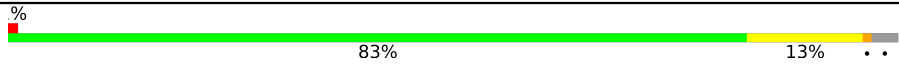
Metric	Percentile Ranks	Value
Rfree		0.221
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		0.9%
RSRZ outliers		1.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	452	% 80% 19% •
1	B	452	% 85% 13% ••
1	C	452	% 84% 13% ••
1	D	452	2% 79% 18% ••
1	E	452	% 82% 15% •

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Mol	Chain	Length	Quality of chain
1	F	452	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 20947 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	2	0
			3412	2157	580	658	17			
1	B	447	Total	C	N	O	S	0	0	0
			3421	2162	586	656	17			
1	C	444	Total	C	N	O	S	0	0	0
			3398	2148	582	651	17			
1	D	440	Total	C	N	O	S	0	2	0
			3390	2146	577	650	17			
1	E	440	Total	C	N	O	S	0	0	0
			3375	2134	580	644	17			
1	F	439	Total	C	N	O	S	0	1	0
			3367	2128	574	648	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	ARG	-	expression tag	UNP B6KCK6
A	446	SER	-	expression tag	UNP B6KCK6
A	447	HIS	-	expression tag	UNP B6KCK6
A	448	HIS	-	expression tag	UNP B6KCK6
A	449	HIS	-	expression tag	UNP B6KCK6
A	450	HIS	-	expression tag	UNP B6KCK6
A	451	HIS	-	expression tag	UNP B6KCK6
A	452	HIS	-	expression tag	UNP B6KCK6
B	445	ARG	-	expression tag	UNP B6KCK6
B	446	SER	-	expression tag	UNP B6KCK6
B	447	HIS	-	expression tag	UNP B6KCK6
B	448	HIS	-	expression tag	UNP B6KCK6
B	449	HIS	-	expression tag	UNP B6KCK6
B	450	HIS	-	expression tag	UNP B6KCK6
B	451	HIS	-	expression tag	UNP B6KCK6
B	452	HIS	-	expression tag	UNP B6KCK6
C	445	ARG	-	expression tag	UNP B6KCK6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	-	expression tag	UNP B6KCK6
C	447	HIS	-	expression tag	UNP B6KCK6
C	448	HIS	-	expression tag	UNP B6KCK6
C	449	HIS	-	expression tag	UNP B6KCK6
C	450	HIS	-	expression tag	UNP B6KCK6
C	451	HIS	-	expression tag	UNP B6KCK6
C	452	HIS	-	expression tag	UNP B6KCK6
D	445	ARG	-	expression tag	UNP B6KCK6
D	446	SER	-	expression tag	UNP B6KCK6
D	447	HIS	-	expression tag	UNP B6KCK6
D	448	HIS	-	expression tag	UNP B6KCK6
D	449	HIS	-	expression tag	UNP B6KCK6
D	450	HIS	-	expression tag	UNP B6KCK6
D	451	HIS	-	expression tag	UNP B6KCK6
D	452	HIS	-	expression tag	UNP B6KCK6
E	445	ARG	-	expression tag	UNP B6KCK6
E	446	SER	-	expression tag	UNP B6KCK6
E	447	HIS	-	expression tag	UNP B6KCK6
E	448	HIS	-	expression tag	UNP B6KCK6
E	449	HIS	-	expression tag	UNP B6KCK6
E	450	HIS	-	expression tag	UNP B6KCK6
E	451	HIS	-	expression tag	UNP B6KCK6
E	452	HIS	-	expression tag	UNP B6KCK6
F	445	ARG	-	expression tag	UNP B6KCK6
F	446	SER	-	expression tag	UNP B6KCK6
F	447	HIS	-	expression tag	UNP B6KCK6
F	448	HIS	-	expression tag	UNP B6KCK6
F	449	HIS	-	expression tag	UNP B6KCK6
F	450	HIS	-	expression tag	UNP B6KCK6
F	451	HIS	-	expression tag	UNP B6KCK6
F	452	HIS	-	expression tag	UNP B6KCK6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total 1	Cl 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is water.

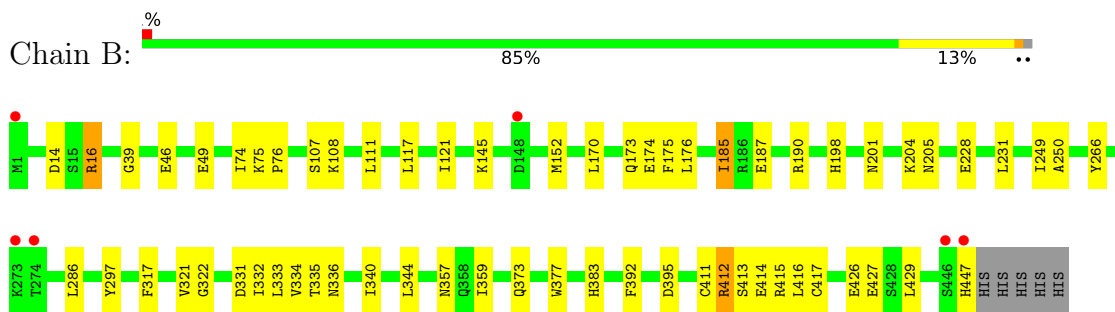| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total 119	O 119	0	0
4	B	99	Total 99	O 99	0	0
4	C	116	Total 116	O 116	0	0
4	D	93	Total 93	O 93	0	0
4	E	86	Total 86	O 86	0	0
4	F	65	Total 65	O 65	0	0

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.
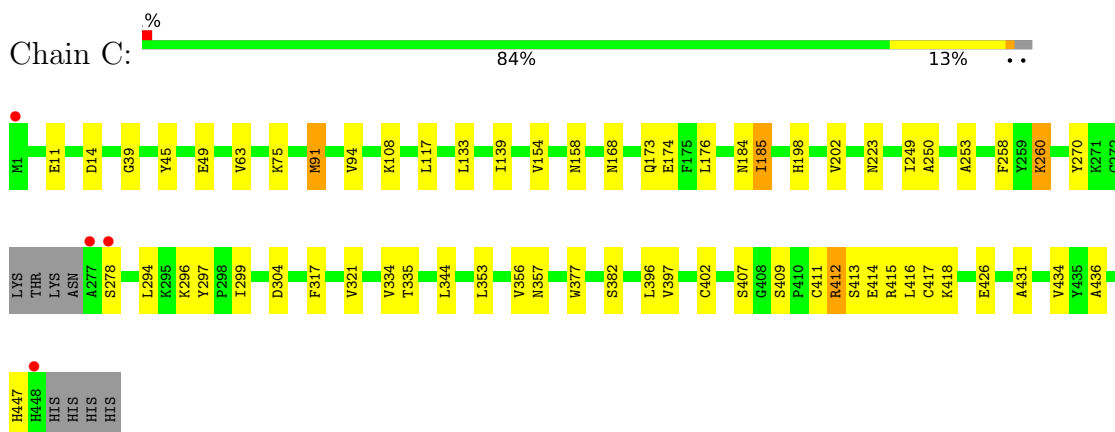
- Molecule 1: Enolase

Chain A:

- Molecule 1: Enolase

Chain B:

- Molecule 1: Enolase

Chain C:

• Molecule 1: Enolase

Chain D:
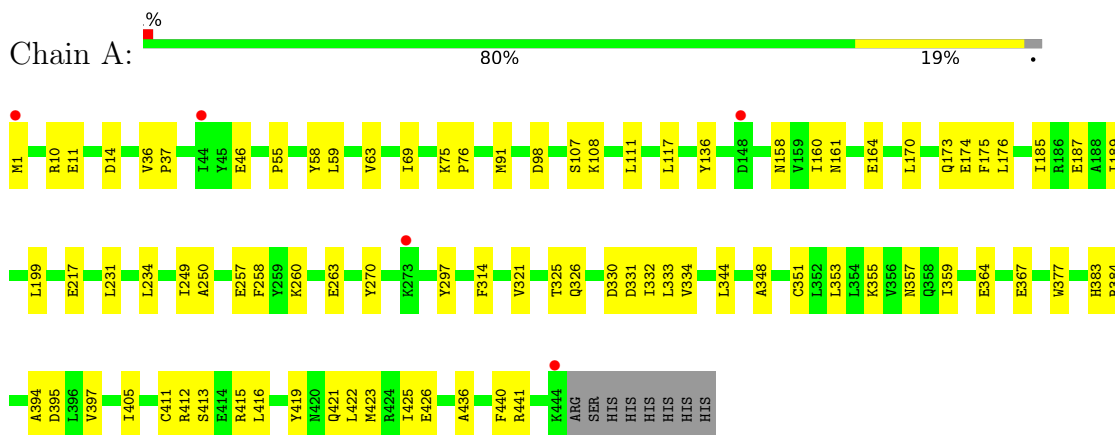
• Molecule 1: Enolase

Chain E:

• Molecule 1: Enolase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	323.63Å　　323.63Å　　66.77Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	29.55　–　2.75 29.55　–　2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.55-2.75) 100.0 (29.55-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.171　,　0.219 0.175　,　0.221	Depositor DCC
R_{free} test set	4548 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20947	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 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CL

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	0.37	0/3467	0.62	0/4674
1	B	0.39	0/3477	0.64	0/4687
1	C	0.38	0/3454	0.64	0/4656
1	D	0.38	0/3446	0.61	0/4646
1	E	0.37	1/3430 (0.0%)	0.61	0/4619
1	F	0.37	0/3420	0.63	0/4607
All	All	0.38	1/20694 (0.0%)	0.63	0/27889

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	417	CYS	CB-SG	-5.07	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3412	0	3444	73	0
1	B	3421	0	3459	50	0
1	C	3398	0	3426	49	0
1	D	3390	0	3416	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3375	0	3396	53	0
1	F	3367	0	3393	47	0
2	E	1	0	0	0	0
3	F	5	0	0	0	0
4	A	119	0	0	2	0
4	B	99	0	0	1	0
4	C	116	0	0	1	0
4	D	93	0	0	2	0
4	E	86	0	0	1	0
4	F	65	0	0	0	0
All	All	20947	0	20534	304	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 7.

All (304) 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:A:321:VAL:HG12	1:A:325:THR:HB	1.37	1.02
1:C:14:ASP:O	1:D:416:LEU:HD13	1.77	0.84
1:E:158:ASN:O	1:E:409:SER:HB3	1.77	0.82
1:C:14:ASP:O	1:D:416:LEU:CD1	2.28	0.81
1:A:423:MET:HE1	4:B:543:HOH:O	1.79	0.80
1:B:201:ASN:HB2	1:C:431:ALA:HB3	1.62	0.80
1:A:334:VAL:HG12	1:A:334:VAL:O	1.83	0.78
1:B:117:LEU:HD22	1:B:357:ASN:HA	1.64	0.78
1:A:14:ASP:O	1:B:416:LEU:HD13	1.84	0.77
1:D:414:GLU:HG2	1:D:415:ARG:HD2	1.65	0.76
1:C:117:LEU:HD22	1:C:357:ASN:HA	1.68	0.75
1:A:321:VAL:CG1	1:A:325:THR:HB	2.17	0.75
1:E:117:LEU:HD22	1:E:357:ASN:HA	1.67	0.74
1:B:46:GLU:HB3	1:B:334:VAL:CG1	2.17	0.73
1:E:416:LEU:HD13	1:F:14:ASP:O	1.89	0.73
1:E:335:THR:O	1:E:335:THR:HG22	1.90	0.71
1:B:334:VAL:HG12	1:B:334:VAL:O	1.90	0.71
1:D:108:LYS:HE3	1:D:359:ILE:O	1.90	0.71
1:E:185:ILE:HG22	1:E:426:GLU:CD	2.11	0.71
1:C:45:TYR:HB2	1:C:334:VAL:HG21	1.73	0.70
1:C:416:LEU:CD1	1:D:14:ASP:O	2.39	0.69
1:A:1:MET:HE1	4:A:546:HOH:O	1.91	0.69
1:B:108:LYS:NZ	1:B:359:ILE:O	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:MET:HE1	1:D:429:LEU:HD12	1.75	0.69
1:B:145:LYS:NZ	1:B:373:GLN:OE1	2.20	0.69
1:E:108:LYS:NZ	1:E:359:ILE:O	2.22	0.69
1:C:414:GLU:HG2	1:C:415:ARG:HD2	1.75	0.68
1:A:416:LEU:HD13	1:B:14:ASP:O	1.94	0.67
1:F:171:ALA:HB2	1:F:268:LEU:O	1.95	0.67
1:D:353:LEU:HD11	1:D:382:SER:HB2	1.76	0.67
1:E:414:GLU:HG2	1:E:415:ARG:HD2	1.77	0.66
1:F:117:LEU:HD22	1:F:357:ASN:HA	1.76	0.65
1:C:260:LYS:HE3	1:C:260:LYS:HA	1.79	0.65
1:C:416:LEU:HD13	1:D:14:ASP:O	1.97	0.64
1:A:185:ILE:HD11	1:A:422:LEU:HD13	1.80	0.63
1:A:117:LEU:HD22	1:A:357:ASN:HA	1.79	0.63
1:B:204:LYS:HD2	1:C:431:ALA:HB1	1.80	0.63
1:F:414:GLU:HG2	1:F:415:ARG:HD2	1.81	0.63
1:C:317:PHE:O	1:C:321:VAL:HG22	1.98	0.63
1:A:46:GLU:HB3	1:A:334:VAL:CG1	2.29	0.63
1:A:136:TYR:CD1	1:A:425:ILE:HD12	2.34	0.63
1:F:74:ILE:HG21	1:F:119:VAL:HG21	1.80	0.63
1:E:168:ASN:O	1:E:271:LYS:HE2	1.99	0.63
1:B:74:ILE:HD11	1:B:111:LEU:HD13	1.80	0.62
1:C:45:TYR:CB	1:C:334:VAL:HG21	2.29	0.62
1:C:407:SER:O	1:C:415:ARG:HG3	1.99	0.62
1:D:75:LYS:HB3	1:D:76:PRO:HD3	1.82	0.61
1:F:176:LEU:N	1:F:176:LEU:HD12	2.14	0.61
1:D:164:GLU:HG2	1:D:257:GLU:HG2	1.83	0.61
1:E:416:LEU:CD1	1:F:14:ASP:O	2.48	0.61
1:A:321:VAL:HG12	1:A:325:THR:CB	2.22	0.60
1:D:176:LEU:N	1:D:176:LEU:HD12	2.16	0.60
1:B:152:MET:HE1	1:B:429:LEU:HD12	1.82	0.60
1:D:117:LEU:HD22	1:D:357:ASN:HA	1.83	0.60
1:B:39:GLY:N	1:B:49:GLU:OE2	2.33	0.60
1:A:11:GLU:HG3	1:A:63:VAL:HG22	1.82	0.60
1:A:75:LYS:HB3	1:A:76:PRO:HD3	1.84	0.59
1:B:173:GLN:HG2	1:B:174:GLU:HG3	1.84	0.59
1:E:359:ILE:CD1	1:E:364:GLU:HB3	2.33	0.59
1:A:55:PRO:HD3	1:C:133:LEU:HD23	1.85	0.58
1:A:173:GLN:HG2	1:A:174:GLU:HG3	1.83	0.58
1:E:173:GLN:HG2	1:E:174:GLU:HG3	1.86	0.58
1:B:331:ASP:O	1:B:334:VAL:HG23	2.03	0.58
1:E:389:GLU:O	1:E:417:CYS:SG	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:SER:HB2	1:E:410:PRO:HD2	1.85	0.58
1:A:421:GLN:O	1:A:425:ILE:HG12	2.03	0.58
1:C:173:GLN:HG2	1:C:174:GLU:HG3	1.85	0.58
1:A:170:LEU:HD21	1:A:175:PHE:CE2	2.40	0.57
1:D:185:ILE:HG22	1:D:426:GLU:CD	2.24	0.57
1:C:39:GLY:N	1:C:49:GLU:OE2	2.37	0.57
1:E:304:ASP:OD2	1:E:330:ASP:HB3	2.05	0.56
1:F:407:SER:O	1:F:415:ARG:HG3	2.06	0.56
1:A:158:ASN:HD21	1:A:161:ASN:HD21	1.52	0.56
1:D:91:MET:HE2	1:D:91:MET:HA	1.87	0.56
1:F:69:ILE:HD13	1:F:111:LEU:HA	1.88	0.56
1:F:91:MET:HE2	1:F:91:MET:HA	1.87	0.56
1:B:46:GLU:HB3	1:B:334:VAL:HG11	1.88	0.55
1:E:366:ILE:HG12	1:E:400:LEU:HD21	1.88	0.55
1:F:75:LYS:HB3	1:F:76:PRO:HD3	1.87	0.55
1:E:171:ALA:HB2	1:E:268:LEU:O	2.07	0.55
1:F:98:ASP:HB2	1:F:111:LEU:HD13	1.89	0.55
1:C:344:LEU:HD23	1:C:377:TRP:CZ2	2.41	0.55
1:D:231:LEU:HD13	1:D:297:TYR:CD2	2.40	0.55
1:E:413:SER:O	1:E:417:CYS:HB2	2.07	0.55
1:E:172:LEU:HD12	1:E:175:PHE:CZ	2.42	0.55
1:A:185:ILE:CD1	1:A:422:LEU:HD13	2.37	0.55
1:B:16:ARG:HG3	1:B:16:ARG:HH11	1.71	0.55
1:E:441:ARG:HG2	4:E:468:HOH:O	2.06	0.55
1:A:164:GLU:HG2	1:A:257:GLU:HG2	1.88	0.54
1:F:185:ILE:HG22	1:F:426:GLU:CD	2.27	0.54
1:B:383:HIS:HD2	1:B:415:ARG:NH1	2.05	0.54
1:A:69:ILE:CG2	1:A:111:LEU:HD22	2.38	0.54
1:F:244[A]:GLU:H	1:F:244[A]:GLU:CD	2.10	0.54
1:A:176:LEU:N	1:A:176:LEU:HD12	2.22	0.54
1:F:244[A]:GLU:OE1	1:F:244[A]:GLU:N	2.32	0.54
1:B:185:ILE:HG22	1:B:426:GLU:CD	2.28	0.53
1:A:383:HIS:HD2	1:A:415:ARG:NH1	2.06	0.53
1:F:332:ILE:HG23	1:F:333:LEU:HG	1.90	0.53
1:B:176:LEU:N	1:B:176:LEU:HD12	2.24	0.53
1:D:294:LEU:HD23	1:D:299:ILE:HB	1.90	0.53
1:A:185:ILE:HD13	1:A:422:LEU:HB3	1.91	0.53
1:E:359:ILE:HD13	1:E:364:GLU:HB3	1.90	0.53
1:F:172:LEU:HD12	1:F:175:PHE:CZ	2.44	0.53
1:D:6:ASP:OD1	1:D:75:LYS:NZ	2.42	0.52
1:D:258:PHE:HB3	1:D:270:TYR:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD23	1:C:377:TRP:CE2	2.44	0.52
1:A:46:GLU:HB3	1:A:334:VAL:HG11	1.92	0.52
1:D:323:GLU:OE1	1:D:323:GLU:N	2.33	0.52
1:E:136:TYR:HE2	1:E:429:LEU:HD21	1.73	0.52
1:B:205:ASN:OD1	1:C:431:ALA:HB2	2.09	0.52
1:D:93:MET:CE	1:D:116:ILE:HG23	2.40	0.52
1:E:413:SER:HB2	1:F:414:GLU:HB3	1.92	0.52
1:D:48:LEU:HD13	1:D:109:SER:HA	1.90	0.52
1:E:185:ILE:O	1:E:185:ILE:HD13	2.10	0.52
1:D:436:ALA:HB1	1:D:440:PHE:HA	1.92	0.51
1:B:117:LEU:HD22	1:B:357:ASN:CA	2.40	0.51
1:D:48:LEU:HD23	1:D:49:GLU:N	2.25	0.51
1:E:407:SER:O	1:E:415:ARG:HG3	2.10	0.51
1:A:55:PRO:HD3	1:C:133:LEU:CD2	2.41	0.51
1:A:160:ILE:HD11	1:A:199:LEU:HD21	1.91	0.51
1:D:50:LEU:CD2	1:D:69:ILE:HD12	2.40	0.51
1:B:413:SER:O	1:B:417:CYS:HB2	2.10	0.51
1:C:335:THR:O	1:C:335:THR:HG22	2.10	0.51
1:B:16:ARG:HG3	1:B:16:ARG:NH1	2.26	0.51
1:B:344:LEU:HD23	1:B:377:TRP:CE2	2.46	0.51
1:A:321:VAL:CG1	1:A:325:THR:CB	2.88	0.51
1:E:14:ASP:O	1:F:416:LEU:CD1	2.59	0.51
1:E:45:TYR:HB2	1:E:334:VAL:HG11	1.93	0.51
1:D:96:GLN:N	1:D:96:GLN:OE1	2.44	0.50
1:C:185:ILE:HG22	1:C:426:GLU:CD	2.31	0.50
1:A:334:VAL:O	1:A:334:VAL:CG1	2.56	0.50
1:D:11:GLU:HG3	1:D:63:VAL:HG22	1.93	0.50
1:A:330:ASP:CG	1:A:353:LEU:HD23	2.31	0.50
1:A:185:ILE:HG22	1:A:426:GLU:CD	2.31	0.50
1:B:228:GLU:N	1:B:228:GLU:OE1	2.39	0.50
1:D:145:LYS:NZ	1:D:400:LEU:O	2.45	0.50
1:D:261:GLN:CD	1:D:261:GLN:H	2.15	0.50
1:F:366:ILE:HG12	1:F:400:LEU:HD21	1.94	0.50
1:B:447:HIS:HD2	1:F:73:GLU:HG3	1.77	0.50
1:F:91:MET:HA	1:F:91:MET:CE	2.41	0.50
1:B:231:LEU:HD13	1:B:297:TYR:CD2	2.47	0.49
1:E:389:GLU:OE1	1:E:389:GLU:N	2.38	0.49
1:A:14:ASP:O	1:B:416:LEU:CD1	2.57	0.49
1:E:75:LYS:HB3	1:E:76:PRO:HD3	1.95	0.49
1:D:407:SER:O	1:D:415:ARG:HG3	2.13	0.49
1:E:413:SER:CB	1:F:414:GLU:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:THR:HG22	1:F:335:THR:O	2.13	0.49
1:E:14:ASP:O	1:F:416:LEU:HD13	2.12	0.49
1:E:394:ALA:O	1:E:397:VAL:HG12	2.12	0.49
1:F:434:VAL:HG12	1:F:435:TYR:N	2.28	0.49
1:D:152:MET:CE	1:D:429:LEU:HD12	2.43	0.49
1:B:411:CYS:O	1:B:412:ARG:HB2	2.13	0.48
1:F:100:THR:HG21	1:F:110:LYS:HG3	1.95	0.48
1:A:416:LEU:CD1	1:B:14:ASP:O	2.59	0.48
1:A:249:ILE:HG22	1:A:250:ALA:N	2.28	0.48
1:D:411:CYS:O	1:D:412:ARG:HB2	2.13	0.48
1:B:335:THR:HG22	1:B:335:THR:O	2.13	0.48
1:A:326:GLN:NE2	1:A:351:CYS:SG	2.86	0.48
1:D:294:LEU:CD1	1:D:321:VAL:HG11	2.43	0.48
1:A:332:ILE:HG23	1:A:333:LEU:HG	1.94	0.48
1:A:394:ALA:O	1:A:397:VAL:HG12	2.13	0.48
1:C:91:MET:HE2	1:C:91:MET:HA	1.95	0.48
1:D:315:SER:O	1:D:319:LYS:HB2	2.13	0.48
1:A:187:GLU:HA	1:A:187:GLU:OE1	2.13	0.48
1:C:11:GLU:HG3	1:C:63:VAL:HG22	1.96	0.48
1:E:353:LEU:HD11	1:E:382:SER:HB2	1.96	0.48
1:B:170:LEU:HD21	1:B:175:PHE:HE2	1.78	0.48
1:C:154:VAL:HG23	1:C:436:ALA:HB3	1.96	0.48
1:A:58:TYR:CE2	1:B:190:ARG:HG3	2.49	0.47
1:C:176:LEU:HD12	1:C:176:LEU:N	2.29	0.47
1:E:11:GLU:HG3	1:E:63:VAL:HG22	1.95	0.47
1:F:98:ASP:CB	1:F:111:LEU:HD13	2.44	0.47
1:E:354:LEU:C	1:E:354:LEU:HD23	2.35	0.47
1:A:98:ASP:OD2	1:A:108:LYS:HA	2.15	0.47
1:A:441:ARG:HG2	4:A:481:HOH:O	2.13	0.47
1:A:36:VAL:HG12	1:A:37:PRO:O	2.14	0.47
1:D:48:LEU:HD23	1:D:49:GLU:C	2.35	0.47
1:A:170:LEU:HD21	1:A:175:PHE:HE2	1.79	0.47
1:A:258:PHE:HB3	1:A:270:TYR:CD2	2.49	0.47
1:A:314:PHE:HB3	1:A:348:ALA:O	2.14	0.47
1:F:326:GLN:NE2	1:F:351:CYS:SG	2.87	0.47
1:D:344:LEU:HD23	1:D:377:TRP:NE1	2.30	0.47
1:D:185:ILE:HG22	1:D:426:GLU:OE1	2.15	0.47
1:A:359:ILE:CD1	1:A:364:GLU:HB3	2.45	0.47
1:B:170:LEU:HD21	1:B:175:PHE:CE2	2.50	0.47
1:E:176:LEU:HD12	1:E:176:LEU:N	2.29	0.47
1:C:91:MET:HA	1:C:91:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD21	1:B:198:HIS:CE1	2.51	0.46
1:A:160:ILE:HB	1:A:175:PHE:HB2	1.98	0.46
1:C:434:VAL:HG21	1:C:447:HIS:HA	1.96	0.46
1:A:69:ILE:HG23	1:A:111:LEU:HD22	1.97	0.46
1:E:408:GLY:HA3	1:E:415:ARG:HG2	1.97	0.46
1:F:319:LYS:O	1:F:319:LYS:HD3	2.15	0.46
1:D:384:ARG:O	1:D:415:ARG:NH2	2.48	0.46
1:A:260:LYS:HB3	1:A:263[A]:GLU:OE1	2.16	0.46
1:D:266:TYR:CG	1:D:286:LEU:HD22	2.51	0.46
1:A:263[A]:GLU:CD	1:A:263[A]:GLU:H	2.17	0.46
1:A:364:GLU:HA	1:A:367[A]:GLU:HG2	1.98	0.46
1:C:94:VAL:HG22	1:C:108:LYS:HD3	1.97	0.46
1:C:249:ILE:HG22	1:C:250:ALA:N	2.30	0.46
1:D:335:THR:HG23	1:D:354:LEU:HD12	1.97	0.46
1:F:411:CYS:O	1:F:412:ARG:HB2	2.15	0.46
1:B:185:ILE:HG22	1:B:426:GLU:OE1	2.16	0.45
1:D:408:GLY:HA3	1:D:415:ARG:HG2	1.99	0.45
1:A:411:CYS:O	1:A:412:ARG:HB2	2.16	0.45
1:B:75:LYS:HB3	1:B:76:PRO:HD3	1.96	0.45
1:D:189:ILE:HD13	1:D:419:TYR:HB3	1.98	0.45
1:E:43:GLY:HA3	1:E:308:GLN:HE22	1.82	0.45
1:F:249:ILE:HG22	1:F:250:ALA:N	2.32	0.45
1:A:331:ASP:O	1:A:334:VAL:HG23	2.17	0.45
1:A:397:VAL:HG21	1:A:405:ILE:HB	1.99	0.45
1:B:121:ILE:HG23	1:B:392:PHE:CD1	2.52	0.45
1:D:401:ARG:NH2	1:D:444:LYS:O	2.50	0.45
1:B:187:GLU:OE1	1:B:187:GLU:HA	2.17	0.45
1:C:413:SER:OG	1:D:414:GLU:HB3	2.17	0.44
1:D:158:ASN:HD21	1:D:174:GLU:HB2	1.81	0.44
1:E:185:ILE:HG22	1:E:426:GLU:OE1	2.16	0.44
1:A:36:VAL:HG13	1:A:117:LEU:HD23	1.99	0.44
1:E:413:SER:OG	1:F:414:GLU:HB3	2.17	0.44
1:F:11:GLU:HG3	1:F:63:VAL:HG22	1.99	0.44
1:F:353:LEU:HD11	1:F:382:SER:HB2	1.99	0.44
1:B:249:ILE:HG22	1:B:250:ALA:N	2.32	0.44
1:F:396:LEU:HD11	1:F:400:LEU:HD11	2.00	0.44
1:C:185:ILE:HG22	1:C:426:GLU:OE1	2.16	0.44
1:D:101:LYS:HA	1:D:107:SER:H	1.83	0.44
1:E:260:LYS:O	1:E:264:LYS:N	2.50	0.44
1:B:317:PHE:O	1:B:321:VAL:HG22	2.17	0.44
1:C:253:ALA:HB3	1:C:304:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ARG:NE	4:D:509:HOH:O	2.32	0.44
1:E:158:ASN:HD21	1:E:161:ASN:HD21	1.66	0.44
1:E:251:PHE:HE1	1:E:299:ILE:HD13	1.83	0.44
1:A:10:ARG:NH1	1:B:427:GLU:OE1	2.51	0.44
1:C:184:ASN:HB2	1:C:426:GLU:OE2	2.18	0.43
1:C:353:LEU:HD11	1:C:382:SER:HB2	2.01	0.43
1:D:44:ILE:HG23	1:D:45:TYR:N	2.33	0.43
1:B:344:LEU:HD23	1:B:377:TRP:CZ2	2.54	0.43
1:E:189:ILE:HD13	1:E:419:TYR:HB3	1.99	0.43
1:E:329:GLY:O	1:E:333:LEU:HD12	2.19	0.43
1:D:294:LEU:HD12	1:D:321:VAL:HG11	1.99	0.43
1:D:344:LEU:HD23	1:D:377:TRP:CE2	2.53	0.43
1:F:189:ILE:HD12	1:F:423:MET:CG	2.49	0.43
1:A:11:GLU:HG3	1:A:63:VAL:CG2	2.47	0.43
1:B:107:SER:O	1:B:108:LYS:HB2	2.19	0.43
1:D:87:LYS:HB2	4:D:477:HOH:O	2.18	0.43
1:E:28:GLU:OE1	1:E:28:GLU:N	2.38	0.43
1:F:327:VAL:O	1:F:349:CYS:HB2	2.19	0.43
1:B:266:TYR:CG	1:B:286:LEU:HD22	2.53	0.43
1:C:296:LYS:HD2	1:C:297:TYR:CZ	2.54	0.43
1:D:91:MET:HA	1:D:91:MET:CE	2.49	0.43
1:D:174:GLU:HG2	1:D:252:ASP:HB3	2.00	0.43
1:F:117:LEU:HD22	1:F:357:ASN:CA	2.48	0.43
1:C:417:CYS:SG	1:C:418:LYS:HD2	2.58	0.42
1:E:44:ILE:HG12	1:E:44:ILE:O	2.19	0.42
1:B:447:HIS:ND1	1:F:72:GLN:OE1	2.53	0.42
1:D:152:MET:CE	1:D:426:GLU:HA	2.50	0.42
1:D:244[B]:GLU:CD	1:D:244[B]:GLU:H	2.22	0.42
1:F:436:ALA:HB1	1:F:440:PHE:HA	2.02	0.42
1:A:58:TYR:CZ	1:B:190:ARG:HG3	2.54	0.42
1:B:336:ASN:O	1:B:340:ILE:HG13	2.18	0.42
1:E:416:LEU:HD12	1:F:15:SER:HA	2.01	0.42
1:C:168:ASN:HB3	1:C:223:ASN:HA	2.01	0.42
1:C:411:CYS:O	1:C:412:ARG:HB2	2.19	0.42
1:C:294:LEU:HD23	1:C:299:ILE:HB	2.02	0.42
1:F:231:LEU:HD13	1:F:297:TYR:CD2	2.55	0.42
1:A:383:HIS:HD2	1:A:415:ARG:HH11	1.68	0.42
1:E:87:LYS:HD2	1:E:363:THR:HG21	2.00	0.42
1:C:414:GLU:HB3	1:D:413:SER:HB2	2.00	0.42
1:A:46:GLU:HB3	1:A:334:VAL:HG13	1.99	0.42
1:A:158:ASN:HD22	1:A:217:GLU:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HD13	1:A:419:TYR:HB3	2.01	0.41
1:B:332:ILE:HG23	1:B:333:LEU:HG	2.02	0.41
1:D:48:LEU:HD23	1:D:48:LEU:C	2.40	0.41
1:C:356:VAL:HG23	4:C:463:HOH:O	2.21	0.41
1:F:185:ILE:HG22	1:F:426:GLU:OE1	2.20	0.41
1:A:189:ILE:HD12	1:A:423:MET:CG	2.50	0.41
1:A:436:ALA:HB1	1:A:440:PHE:HA	2.03	0.41
1:D:137:LYS:HD3	1:D:147:ILE:HD12	2.02	0.41
1:A:231:LEU:HD13	1:A:297:TYR:CD2	2.56	0.41
1:A:344:LEU:HD23	1:A:377:TRP:CE2	2.55	0.41
1:A:355:LYS:HD3	1:A:384:ARG:NE	2.35	0.41
1:C:117:LEU:HD22	1:C:357:ASN:CA	2.46	0.41
1:C:158:ASN:O	1:C:409:SER:OG	2.20	0.41
1:C:397:VAL:HG23	1:C:402:CYS:HB2	2.02	0.41
1:A:325:THR:HG22	1:A:326:GLN:N	2.34	0.41
1:C:249:ILE:CG2	1:C:250:ALA:N	2.84	0.41
1:D:81:LYS:NZ	1:E:244:GLU:OE2	2.54	0.41
1:D:159:VAL:HG22	1:D:175:PHE:O	2.20	0.41
1:E:411:CYS:O	1:E:412:ARG:HB2	2.21	0.41
1:C:198:HIS:O	1:C:202:VAL:HG23	2.21	0.41
1:D:336:ASN:O	1:D:340:ILE:HG13	2.21	0.41
1:F:198:HIS:O	1:F:202:VAL:HG23	2.20	0.41
1:A:175:PHE:HB3	1:A:234:LEU:HD11	2.03	0.41
1:D:152:MET:HE3	1:D:425:ILE:HG22	2.02	0.41
1:D:330:ASP:CG	1:D:353:LEU:HD23	2.41	0.41
1:D:335:THR:HG22	1:D:335:THR:O	2.21	0.41
1:E:383:HIS:CG	1:E:407:SER:HA	2.56	0.41
1:F:314:PHE:HB3	1:F:348:ALA:O	2.21	0.41
1:F:152:MET:HE2	1:F:185:ILE:HG21	2.03	0.41
1:C:139:ILE:HG21	1:C:396:LEU:HD12	2.03	0.40
1:A:107:SER:O	1:A:108:LYS:HB2	2.20	0.40
1:A:413:SER:OG	1:B:414:GLU:HB3	2.22	0.40
1:C:258:PHE:HB3	1:C:270:TYR:CD2	2.56	0.40
1:E:262:ASP:OD1	1:E:262:ASP:N	2.54	0.40
1:E:408:GLY:HA3	1:E:415:ARG:CG	2.51	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	444/452 (98%)	432 (97%)	12 (3%)	0	100	100
1	B	445/452 (98%)	420 (94%)	23 (5%)	2 (0%)	34	53
1	C	440/452 (97%)	422 (96%)	16 (4%)	2 (0%)	29	47
1	D	438/452 (97%)	413 (94%)	25 (6%)	0	100	100
1	E	432/452 (96%)	413 (96%)	18 (4%)	1 (0%)	47	69
1	F	434/452 (96%)	414 (95%)	18 (4%)	2 (0%)	29	47
All	All	2633/2712 (97%)	2514 (96%)	112 (4%)	7 (0%)	41	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	SER
1	F	255	ALA
1	F	412	ARG
1	B	412	ARG
1	C	412	ARG
1	E	223	ASN
1	B	322	GLY

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	362/368 (98%)	360 (99%)	2 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	B	363/368 (99%)	360 (99%)	3 (1%)		81	88
1	C	360/368 (98%)	356 (99%)	4 (1%)		73	84
1	D	359/368 (98%)	354 (99%)	5 (1%)		67	79
1	E	357/368 (97%)	356 (100%)	1 (0%)		92	95
1	F	357/368 (97%)	353 (99%)	4 (1%)		73	84
All	All	2158/2208 (98%)	2139 (99%)	19 (1%)		78	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	MET
1	A	395	ASP
1	B	16	ARG
1	B	185	ILE
1	B	395	ASP
1	C	75	LYS
1	C	91	MET
1	C	185	ILE
1	C	260	LYS
1	D	28	GLU
1	D	96	GLN
1	D	185	ILE
1	D	261	GLN
1	D	395	ASP
1	E	185	ILE
1	F	57	ARG
1	F	185	ILE
1	F	319	LYS
1	F	395	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	96	GLN
1	A	158	ASN
1	A	161	ASN
1	A	232	ASN
1	A	326	GLN

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Mol	Chain	Res	Type
1	A	358	GLN
1	A	380	GLN
1	A	404	GLN
1	B	18	ASN
1	B	72	GLN
1	B	158	ASN
1	B	165	HIS
1	B	232	ASN
1	B	261	GLN
1	B	308	GLN
1	B	358	GLN
1	C	18	ASN
1	C	96	GLN
1	C	161	ASN
1	C	232	ASN
1	C	326	GLN
1	C	358	GLN
1	C	380	GLN
1	C	404	GLN
1	D	18	ASN
1	D	158	ASN
1	D	161	ASN
1	D	165	HIS
1	D	205	ASN
1	D	232	ASN
1	D	261	GLN
1	D	280	HIS
1	D	326	GLN
1	D	358	GLN
1	D	380	GLN
1	D	404	GLN
1	E	18	ASN
1	E	158	ASN
1	E	161	ASN
1	E	232	ASN
1	E	308	GLN
1	F	18	ASN
1	F	86	GLN
1	F	161	ASN
1	F	201	ASN
1	F	232	ASN
1	F	326	GLN

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Mol	Chain	Res	Type
1	F	358	GLN
1	F	380	GLN
1	F	404	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	F	453	-	4,4,4	0.14	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	444/452 (98%)	-0.42	5 (1%)	80	86	29, 42, 59, 79	0
1	B	447/452 (98%)	-0.39	6 (1%)	77	84	29, 41, 61, 91	0
1	C	444/452 (98%)	-0.44	4 (0%)	84	89	28, 40, 61, 113	0
1	D	440/452 (97%)	-0.33	9 (2%)	65	73	29, 45, 71, 100	0
1	E	440/452 (97%)	-0.31	6 (1%)	75	82	32, 46, 72, 92	0
1	F	439/452 (97%)	-0.40	4 (0%)	84	89	30, 43, 62, 99	0
All	All	2654/2712 (97%)	-0.38	34 (1%)	77	84	28, 43, 66, 113	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	ALA	5.1
1	D	1	MET	4.5
1	D	42	THR	4.2
1	B	273	LYS	3.8
1	D	44	ILE	3.8
1	E	1	MET	3.4
1	E	277	ALA	3.3
1	F	1	MET	3.3
1	D	43	GLY	3.3
1	E	262	ASP	3.2
1	F	278	SER	3.0
1	A	273	LYS	3.0
1	E	261	GLN	3.0
1	B	148	ASP	2.9
1	A	1	MET	2.8
1	E	44	ILE	2.7
1	D	147	ILE	2.7
1	C	277	ALA	2.7
1	C	278	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.6
1	D	148	ASP	2.6
1	A	44	ILE	2.5
1	B	274	THR	2.4
1	C	448	HIS	2.4
1	F	446	SER	2.4
1	D	446	SER	2.4
1	B	1	MET	2.2
1	D	39	GLY	2.2
1	B	446	SER	2.2
1	A	148	ASP	2.1
1	A	444	LYS	2.1
1	E	48	LEU	2.0
1	F	431	ALA	2.0
1	B	447	HIS	2.0

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($\mathring{A}^2$)	Q<0.9
2	CL	E	453	1/1	0.95	0.14	64,64,64,64	0
3	SO4	F	453	5/5	0.96	0.24	79,79,80,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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