



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:54 PM GMT

PDB ID : 1Z1W  
Title : Crystal structures of the tricorn interacting facor F3 from *Thermoplasma acidophilum*, a zinc aminopeptidase in three different conformations  
Authors : Kyrieleis, O.J.P.; Goettig, P.; Kiefersauer, R.; Huber, R.; Brandstetter, H.  
Deposited on : 2005-03-07  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

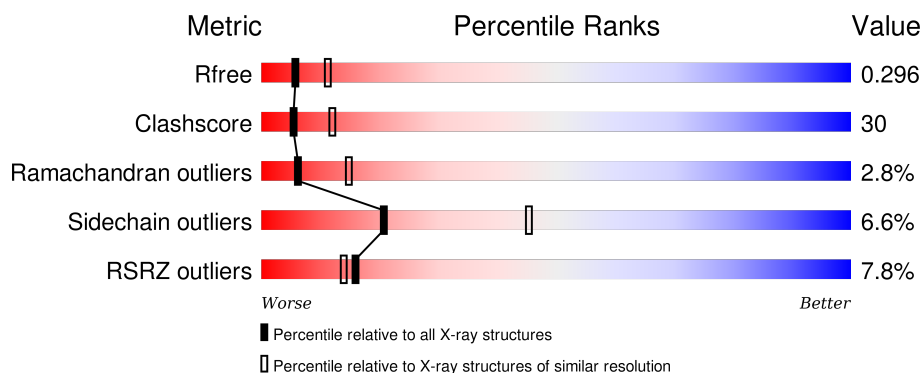
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	780	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6654 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 Tricorn protease interacting factor F3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	145	0	0
			6295	4008	1066	1190	31			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- 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		

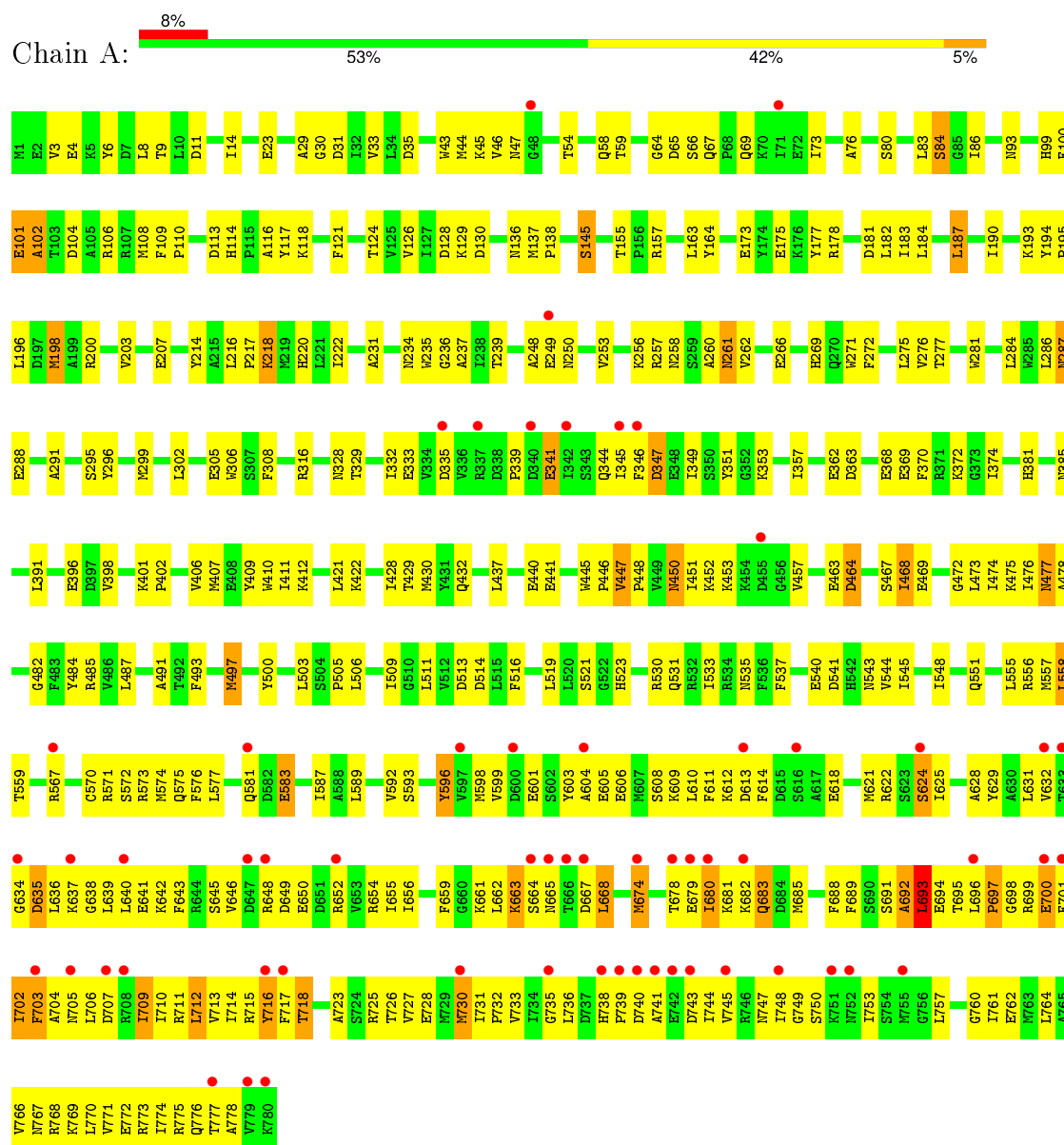
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	353	Total 353	O 353	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Tricorn protease interacting factor F3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.79Å 104.79Å 137.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.70 19.92 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.92-2.70) 98.1 (19.92-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.47 (at 2.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.295 0.222 , 0.296	Depositor DCC
$R_{free}$ test set	1199 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.7	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39763 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.41	1/6429 (0.0%)	0.61	0/8677

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLU	CD-OE2	7.49	1.33	1.25

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	6295	0	6206	363	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	353	0	0	22	0
All	All	6654	0	6206	363	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 30.

All (363) 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:744:ILE:HG21	1:A:761:ILE:HD11	1.24	1.12
1:A:706:LEU:HA	1:A:709:ILE:HG22	1.32	1.12
1:A:432:GLN:HE22	1:A:445:TRP:H	1.09	0.99
1:A:692:ALA:HB1	1:A:702:ILE:HG12	1.48	0.94
1:A:683:GLN:H	1:A:683:GLN:HE21	1.18	0.92
1:A:421:LEU:HD23	1:A:430:MET:HB3	1.53	0.91
1:A:703:PHE:HA	1:A:706:LEU:HB3	1.51	0.89
1:A:136:ASN:HD21	1:A:164:TYR:H	1.19	0.89
1:A:432:GLN:NE2	1:A:445:TRP:H	1.71	0.89
1:A:114:HIS:HD2	1:A:116:ALA:H	1.21	0.88
1:A:477:ASN:HD21	1:A:482:GLY:H	1.21	0.87
1:A:692:ALA:HB1	1:A:702:ILE:CG1	2.07	0.84
1:A:652:ARG:HD3	1:A:681:LYS:HD3	1.59	0.84
1:A:506:LEU:HD23	1:A:509:ILE:HD12	1.61	0.83
1:A:703:PHE:O	1:A:707:ASP:HB2	1.79	0.81
1:A:683:GLN:H	1:A:683:GLN:NE2	1.79	0.81
1:A:541:ASP:O	1:A:545:ILE:HG12	1.82	0.79
1:A:744:ILE:HG21	1:A:761:ILE:CD1	2.11	0.78
1:A:744:ILE:HG23	1:A:757:LEU:HD11	1.65	0.78
1:A:706:LEU:HD13	1:A:713:VAL:HG21	1.66	0.77
1:A:699:ARG:HA	1:A:702:ILE:HD13	1.65	0.77
1:A:574:MET:HE1	1:A:593:SER:HA	1.67	0.76
1:A:636:LEU:O	1:A:640:LEU:HD13	1.86	0.76
1:A:739:PRO:HB3	1:A:768:ARG:HH22	1.49	0.76
1:A:129:LYS:HE2	1:A:145:SER:O	1.86	0.75
1:A:137:MET:HG2	1:A:155:THR:HG22	1.68	0.75
1:A:374:ILE:HD13	1:A:391:LEU:HD11	1.69	0.74
1:A:407:MET:O	1:A:411:ILE:HG12	1.88	0.74
1:A:741:ALA:O	1:A:745:VAL:HG23	1.87	0.74
1:A:332:ILE:HD11	1:A:353:LYS:HG2	1.70	0.73
1:A:738:HIS:HB2	1:A:739:PRO:C	2.09	0.73
1:A:706:LEU:CA	1:A:709:ILE:HG22	2.16	0.73
1:A:136:ASN:HD21	1:A:164:TYR:N	1.87	0.73
1:A:705:ASN:ND2	1:A:709:ILE:HG21	2.04	0.72
1:A:636:LEU:HD22	1:A:667:ASP:HA	1.69	0.72
1:A:284:LEU:HB3	1:A:345:ILE:HG12	1.69	0.72
1:A:369:GLU:HG3	1:A:398:VAL:HG12	1.72	0.72
1:A:635:ASP:OD1	1:A:638:GLY:HA3	1.90	0.72
1:A:333:GLU:OE1	1:A:412:LYS:HG2	1.89	0.72
1:A:136:ASN:ND2	1:A:164:TYR:H	1.86	0.72
1:A:432:GLN:HE22	1:A:445:TRP:N	1.86	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLY:O	1:A:64:GLY:HA3	1.89	0.71
1:A:106:ARG:HH21	1:A:113:ASP:HB3	1.55	0.71
1:A:220:HIS:HB3	1:A:222:ILE:HD11	1.73	0.71
1:A:218:LYS:NZ	1:A:220:HIS:HD2	1.88	0.70
1:A:574:MET:HE2	1:A:596:TYR:HD2	1.57	0.70
1:A:709:ILE:O	1:A:709:ILE:HG23	1.92	0.70
1:A:497:MET:HG2	1:A:535:ASN:ND2	2.06	0.69
1:A:652:ARG:HD3	1:A:681:LYS:CD	2.22	0.69
1:A:505:PRO:O	1:A:509:ILE:HG13	1.93	0.68
1:A:493:PHE:CZ	1:A:497:MET:HE1	2.29	0.68
1:A:738:HIS:HB2	1:A:740:ASP:N	2.09	0.68
1:A:86:ILE:HD13	1:A:108:MET:HE3	1.75	0.68
1:A:497:MET:HE3	1:A:535:ASN:HB2	1.76	0.67
1:A:572:SER:O	1:A:575:GLN:HG3	1.95	0.67
1:A:637:LYS:O	1:A:641:GLU:HG3	1.94	0.67
1:A:138:PRO:HG3	1:A:218:LYS:HG3	1.78	0.66
1:A:732:PRO:HB2	1:A:767:ASN:ND2	2.11	0.66
1:A:712:LEU:HD22	1:A:716:TYR:CE1	2.30	0.66
1:A:650:GLU:HG2	1:A:654:ARG:HH11	1.60	0.66
1:A:726:THR:HG22	1:A:730:MET:SD	2.36	0.66
1:A:703:PHE:N	4:A:806:HOH:O	2.29	0.65
1:A:406:VAL:O	1:A:410:TRP:HD1	1.79	0.65
1:A:422:LYS:HE3	4:A:981:HOH:O	1.96	0.65
1:A:138:PRO:HG3	1:A:218:LYS:CG	2.27	0.65
1:A:574:MET:CE	1:A:593:SER:HA	2.27	0.64
1:A:573:ARG:N	1:A:573:ARG:HD2	2.12	0.64
1:A:622:ARG:HG3	1:A:622:ARG:HH21	1.61	0.64
1:A:14:ILE:H	1:A:14:ILE:HD12	1.62	0.64
1:A:432:GLN:HE22	1:A:445:TRP:HB2	1.62	0.64
1:A:605:GLU:HA	1:A:632:VAL:HG21	1.79	0.64
1:A:642:LYS:HA	1:A:645:SER:OG	1.98	0.63
1:A:249:GLU:HA	1:A:256:LYS:HD3	1.80	0.63
1:A:774:ILE:O	1:A:777:THR:HG22	1.98	0.63
1:A:649:ASP:HB2	1:A:652:ARG:NH1	2.14	0.62
1:A:767:ASN:O	1:A:771:VAL:HG23	1.99	0.62
1:A:650:GLU:HG2	1:A:654:ARG:NH1	2.14	0.62
1:A:699:ARG:CA	1:A:702:ILE:HD13	2.30	0.62
1:A:537:PHE:O	1:A:573:ARG:HD3	2.00	0.62
1:A:683:GLN:HB2	4:A:1050:HOH:O	1.98	0.62
1:A:731:ILE:CD1	1:A:757:LEU:HD12	2.29	0.62
1:A:23:GLU:OE1	1:A:110:PRO:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:CD2	1:A:430:MET:HB3	2.29	0.61
1:A:718:THR:HA	1:A:723:ALA:HB2	1.83	0.61
1:A:603:TYR:HA	1:A:606:GLU:CD	2.20	0.61
1:A:35:ASP:O	1:A:110:PRO:HA	1.99	0.61
1:A:516:PHE:CG	1:A:551:GLN:HG2	2.36	0.61
1:A:231:ALA:HA	1:A:239:THR:O	2.02	0.60
1:A:608:SER:OG	1:A:629:TYR:HA	2.01	0.60
1:A:175:GLU:HB3	1:A:182:LEU:HB2	1.83	0.60
1:A:368:GLU:OE1	1:A:372:LYS:HE3	2.00	0.60
1:A:558:LEU:HD12	1:A:559:THR:HG22	1.83	0.60
1:A:203:VAL:O	1:A:207:GLU:HG3	2.00	0.60
1:A:744:ILE:CG2	1:A:757:LEU:HD11	2.30	0.60
1:A:618:GLU:HG3	4:A:901:HOH:O	2.01	0.60
1:A:429:THR:HG22	1:A:467:SER:HB3	1.84	0.60
1:A:683:GLN:N	1:A:683:GLN:HE21	1.93	0.59
1:A:713:VAL:HA	1:A:716:TYR:CE2	2.36	0.59
1:A:86:ILE:HD13	1:A:108:MET:CE	2.33	0.59
1:A:333:GLU:HB2	1:A:411:ILE:HG22	1.85	0.59
1:A:497:MET:HE3	1:A:535:ASN:CB	2.33	0.59
1:A:556:ARG:NH2	1:A:599:VAL:HG12	2.18	0.58
1:A:674:MET:HB3	1:A:680:ILE:HG12	1.86	0.58
1:A:101:GLU:O	1:A:102:ALA:HB3	2.04	0.58
1:A:695:THR:O	1:A:699:ARG:HB3	2.04	0.57
1:A:106:ARG:NH2	1:A:113:ASP:HB3	2.18	0.57
1:A:731:ILE:HD11	1:A:757:LEU:HD12	1.87	0.57
1:A:577:LEU:HD13	1:A:589:LEU:HA	1.86	0.57
1:A:727:VAL:HG23	1:A:728:GLU:H	1.68	0.57
1:A:175:GLU:HB2	1:A:196:LEU:HD13	1.85	0.57
1:A:727:VAL:HG23	1:A:728:GLU:N	2.20	0.57
1:A:643:PHE:HB2	1:A:655:ILE:HG21	1.86	0.57
1:A:697:PRO:HG2	1:A:698:GLY:H	1.69	0.57
1:A:712:LEU:HD22	1:A:716:TYR:HE1	1.69	0.57
1:A:505:PRO:HG2	4:A:1103:HOH:O	2.05	0.57
1:A:709:ILE:HG23	1:A:713:VAL:HG23	1.86	0.57
1:A:598:MET:CE	1:A:694:GLU:HG2	2.35	0.56
1:A:198:MET:HA	1:A:198:MET:HE3	1.87	0.56
1:A:570:CYS:O	1:A:574:MET:HB2	2.06	0.56
1:A:696:LEU:N	1:A:697:PRO:HD2	2.20	0.56
1:A:506:LEU:HA	1:A:509:ILE:HD12	1.86	0.56
1:A:305:GLU:HB2	4:A:963:HOH:O	2.05	0.56
1:A:506:LEU:HA	1:A:509:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:HIS:HB3	1:A:222:ILE:CD1	2.36	0.56
1:A:705:ASN:HD21	1:A:709:ILE:HD13	1.69	0.55
1:A:181:ASP:HB3	1:A:183:ILE:HD11	1.89	0.55
1:A:396:GLU:HG3	1:A:401:LYS:O	2.06	0.55
1:A:99:HIS:NE2	1:A:101:GLU:HB2	2.22	0.55
1:A:583:GLU:O	1:A:587:ILE:HG12	2.07	0.55
1:A:173:GLU:HG3	1:A:193:LYS:HG2	1.88	0.55
1:A:261:ASN:ND2	1:A:295:SER:OG	2.39	0.55
1:A:218:LYS:HD2	1:A:218:LYS:C	2.28	0.54
1:A:702:ILE:N	1:A:702:ILE:HD12	2.22	0.54
1:A:774:ILE:C	1:A:776:GLN:H	2.11	0.54
1:A:674:MET:HG2	1:A:679:GLU:HB2	1.90	0.54
1:A:422:LYS:HG3	4:A:991:HOH:O	2.08	0.54
1:A:485:ARG:NH1	1:A:513:ASP:OD1	2.41	0.54
1:A:341:GLU:O	1:A:345:ILE:HG22	2.07	0.54
1:A:491:ALA:HB1	4:A:839:HOH:O	2.07	0.54
1:A:703:PHE:CA	1:A:706:LEU:HB3	2.32	0.54
1:A:709:ILE:HD11	1:A:712:LEU:HD12	1.89	0.53
1:A:473:LEU:HD23	1:A:474:ILE:N	2.24	0.53
1:A:341:GLU:HA	1:A:344:GLN:HB3	1.89	0.53
1:A:173:GLU:HB2	1:A:190:ILE:HD13	1.89	0.53
1:A:33:VAL:HG23	1:A:59:THR:HG21	1.90	0.53
1:A:743:ASP:O	1:A:747:ASN:N	2.40	0.53
1:A:709:ILE:CD1	1:A:712:LEU:HD12	2.39	0.53
1:A:692:ALA:CB	1:A:702:ILE:HG12	2.30	0.53
1:A:744:ILE:CG2	1:A:761:ILE:HD11	2.17	0.53
1:A:516:PHE:CD1	1:A:551:GLN:HG2	2.44	0.53
1:A:500:TYR:HA	1:A:503:LEU:CD1	2.39	0.53
1:A:65:ASP:H	1:A:69:GLN:NE2	2.07	0.53
1:A:277:THR:O	1:A:385:ASN:HA	2.09	0.53
1:A:33:VAL:HG23	1:A:59:THR:CG2	2.39	0.52
1:A:622:ARG:HG3	1:A:622:ARG:NH2	2.23	0.52
1:A:253:VAL:CG2	1:A:583:GLU:HG3	2.39	0.52
1:A:711:ARG:O	1:A:715:ARG:HG3	2.09	0.52
1:A:731:ILE:HD12	1:A:760:GLY:HA3	1.91	0.52
1:A:635:ASP:CG	1:A:638:GLY:HA3	2.30	0.52
1:A:31:ASP:HA	1:A:64:GLY:HA3	1.91	0.52
1:A:543:ASN:HA	4:A:874:HOH:O	2.09	0.52
1:A:604:ALA:O	1:A:628:ALA:HB1	2.10	0.52
1:A:700:GLU:O	1:A:704:ALA:HB2	2.10	0.52
1:A:157:ARG:NH2	4:A:918:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:SER:HB2	4:A:817:HOH:O	2.10	0.52
1:A:696:LEU:HD23	1:A:699:ARG:HH12	1.75	0.52
1:A:450:ASN:ND2	1:A:478:ALA:HB3	2.25	0.51
1:A:544:VAL:O	1:A:548:ILE:HG12	2.10	0.51
1:A:649:ASP:HB2	1:A:652:ARG:HH11	1.75	0.51
1:A:349:ILE:O	1:A:353:LYS:HB3	2.10	0.51
1:A:556:ARG:CZ	1:A:599:VAL:HG12	2.40	0.51
1:A:269:HIS:HA	1:A:272:PHE:O	2.11	0.51
1:A:709:ILE:O	1:A:709:ILE:CG2	2.59	0.51
1:A:606:GLU:O	1:A:610:LEU:HG	2.11	0.51
1:A:506:LEU:HD23	1:A:509:ILE:CD1	2.36	0.50
1:A:346:PHE:HA	1:A:351:TYR:CE2	2.46	0.50
1:A:353:LYS:O	1:A:357:ILE:HG23	2.11	0.50
1:A:54:THR:HB	4:A:904:HOH:O	2.10	0.50
1:A:374:ILE:CD1	1:A:391:LEU:HD11	2.40	0.50
1:A:612:LYS:HG3	1:A:613:ASP:OD2	2.11	0.50
1:A:218:LYS:HZ2	1:A:220:HIS:HD2	1.58	0.50
1:A:450:ASN:HD21	1:A:478:ALA:HB3	1.76	0.50
1:A:482:GLY:HA3	1:A:484:TYR:CE2	2.47	0.50
1:A:664:SER:HB3	1:A:667:ASP:CG	2.31	0.50
1:A:738:HIS:CB	1:A:739:PRO:C	2.80	0.50
1:A:198:MET:CE	1:A:198:MET:HA	2.42	0.50
1:A:710:ILE:O	1:A:714:ILE:HD13	2.12	0.50
1:A:118:LYS:HB2	1:A:157:ARG:HH22	1.77	0.49
1:A:452:LYS:HG3	1:A:478:ALA:HB2	1.94	0.49
1:A:661:LYS:NZ	1:A:691:SER:HB2	2.27	0.49
1:A:702:ILE:H	1:A:702:ILE:HD12	1.78	0.49
1:A:712:LEU:O	1:A:715:ARG:HB2	2.12	0.49
1:A:634:GLY:O	1:A:635:ASP:HB2	2.11	0.49
1:A:702:ILE:HG22	1:A:703:PHE:N	2.26	0.49
1:A:735:GLY:HA2	1:A:740:ASP:OD2	2.12	0.49
1:A:114:HIS:CD2	1:A:116:ALA:H	2.13	0.49
1:A:674:MET:SD	1:A:679:GLU:HB2	2.52	0.49
1:A:76:ALA:HB2	4:A:878:HOH:O	2.13	0.49
1:A:121:PHE:CE1	1:A:163:LEU:HD11	2.48	0.49
1:A:649:ASP:HA	1:A:652:ARG:HB2	1.94	0.49
1:A:65:ASP:OD1	1:A:66:SER:O	2.31	0.49
1:A:218:LYS:HZ3	1:A:220:HIS:HD2	1.58	0.49
1:A:557:MET:HG2	1:A:733:VAL:CG1	2.43	0.49
1:A:446:PRO:HA	1:A:463:GLU:HG2	1.95	0.49
1:A:739:PRO:HB3	1:A:768:ARG:NH2	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:HD22	1:A:770:LEU:O	2.13	0.49
1:A:100:PHE:HA	1:A:104:ASP:HB2	1.94	0.49
1:A:674:MET:CB	1:A:680:ILE:HG12	2.43	0.48
1:A:731:ILE:HB	1:A:732:PRO:CD	2.43	0.48
1:A:668:LEU:HB3	4:A:1015:HOH:O	2.13	0.48
1:A:519:LEU:O	1:A:519:LEU:HD22	2.14	0.48
1:A:43:TRP:CZ3	1:A:45:LYS:HE3	2.49	0.48
1:A:637:LYS:NZ	4:A:1149:HOH:O	2.46	0.48
1:A:102:ALA:HA	1:A:281:TRP:CH2	2.49	0.48
1:A:485:ARG:HB3	1:A:514:ASP:CG	2.34	0.48
1:A:530:ARG:O	1:A:533:ILE:HG22	2.13	0.48
1:A:473:LEU:C	1:A:473:LEU:HD23	2.34	0.48
1:A:693:LEU:O	1:A:693:LEU:HD12	2.14	0.48
1:A:257:ARG:HG3	1:A:306:TRP:CD2	2.49	0.48
1:A:475:LYS:HE2	1:A:511:LEU:HD21	1.95	0.47
1:A:46:VAL:O	1:A:47:ASN:HB2	2.14	0.47
1:A:296:TYR:OH	1:A:316:ARG:NH1	2.48	0.47
1:A:509:ILE:HD11	4:A:1002:HOH:O	2.13	0.47
1:A:276:VAL:HG22	1:A:381:HIS:O	2.15	0.47
1:A:706:LEU:O	1:A:706:LEU:HD12	2.15	0.47
1:A:731:ILE:HB	1:A:732:PRO:HD3	1.97	0.47
1:A:682:LYS:HB2	1:A:685:MET:HE2	1.97	0.47
1:A:639:LEU:HD12	1:A:662:LEU:HD11	1.97	0.47
1:A:709:ILE:HG12	1:A:712:LEU:HB2	1.97	0.47
1:A:605:GLU:HG2	1:A:632:VAL:HG13	1.95	0.47
1:A:257:ARG:HG3	1:A:306:TRP:CE3	2.50	0.47
1:A:557:MET:HG2	1:A:733:VAL:HG13	1.97	0.47
1:A:577:LEU:HD13	1:A:589:LEU:CA	2.44	0.46
1:A:500:TYR:HA	1:A:503:LEU:HD12	1.96	0.46
1:A:750:SER:HB3	1:A:753:ILE:HG12	1.96	0.46
1:A:447:VAL:HA	1:A:448:PRO:HD3	1.84	0.46
1:A:696:LEU:HD23	1:A:699:ARG:NH1	2.31	0.46
1:A:663:LYS:HB3	1:A:697:PRO:HB2	1.96	0.46
1:A:118:LYS:HB2	1:A:157:ARG:NH2	2.30	0.46
1:A:605:GLU:HG2	1:A:632:VAL:CG1	2.45	0.46
1:A:299:MET:CE	1:A:302:LEU:HD12	2.45	0.46
1:A:621:MET:O	1:A:625:ILE:HG12	2.14	0.46
1:A:688:PHE:O	1:A:692:ALA:HB2	2.15	0.46
1:A:739:PRO:C	1:A:741:ALA:H	2.19	0.46
1:A:709:ILE:HG12	1:A:712:LEU:HD12	1.98	0.46
1:A:362:GLU:HG3	1:A:370:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LYS:CB	1:A:697:PRO:HB2	2.46	0.46
1:A:299:MET:HE1	1:A:302:LEU:HD12	1.97	0.46
1:A:450:ASN:OD1	1:A:450:ASN:C	2.54	0.45
1:A:521:SER:OG	1:A:523:HIS:HD2	1.98	0.45
1:A:618:GLU:O	1:A:622:ARG:HG2	2.16	0.45
1:A:437:LEU:O	1:A:521:SER:HA	2.17	0.45
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.72	0.45
1:A:731:ILE:HD13	1:A:757:LEU:HD12	1.96	0.45
1:A:682:LYS:O	1:A:685:MET:HG2	2.16	0.45
1:A:540:GLU:HG2	1:A:576:PHE:CZ	2.51	0.45
1:A:741:ALA:HA	1:A:744:ILE:HD12	1.98	0.45
1:A:234:ASN:HB2	1:A:237:ALA:O	2.17	0.45
1:A:257:ARG:HD2	1:A:308:PHE:CE1	2.52	0.45
1:A:702:ILE:HG21	4:A:996:HOH:O	2.16	0.45
1:A:138:PRO:HG3	1:A:218:LYS:HG2	1.96	0.45
1:A:328:ASN:ND2	1:A:762:GLU:OE2	2.50	0.45
1:A:689:PHE:O	1:A:692:ALA:HB3	2.17	0.44
1:A:705:ASN:O	1:A:709:ILE:HB	2.17	0.44
1:A:640:LEU:O	1:A:643:PHE:HB3	2.17	0.44
1:A:83:LEU:O	1:A:84:SER:HB2	2.17	0.44
1:A:655:ILE:HG22	1:A:659:PHE:CZ	2.52	0.44
1:A:762:GLU:O	1:A:766:VAL:HG23	2.16	0.44
1:A:649:ASP:O	1:A:650:GLU:C	2.54	0.44
1:A:570:CYS:HB3	1:A:596:TYR:CD2	2.52	0.44
1:A:571:ARG:HA	1:A:596:TYR:HE2	1.83	0.44
1:A:609:LYS:C	1:A:611:PHE:H	2.21	0.44
1:A:101:GLU:O	1:A:102:ALA:CB	2.65	0.44
1:A:661:LYS:HZ3	1:A:691:SER:HB2	1.82	0.44
1:A:603:TYR:HA	1:A:606:GLU:CG	2.48	0.44
1:A:477:ASN:ND2	1:A:482:GLY:H	2.03	0.44
1:A:682:LYS:NZ	4:A:1030:HOH:O	2.49	0.44
1:A:769:LYS:O	1:A:773:ARG:HG3	2.18	0.44
1:A:693:LEU:HA	1:A:699:ARG:HG3	2.00	0.44
1:A:711:ARG:HG3	1:A:712:LEU:H	1.82	0.44
1:A:748:ILE:HG12	1:A:757:LEU:CD2	2.48	0.43
1:A:509:ILE:CD1	4:A:1002:HOH:O	2.66	0.43
1:A:574:MET:HE1	1:A:593:SER:CA	2.42	0.43
1:A:44:MET:HG3	1:A:73:ILE:HG12	2.00	0.43
1:A:558:LEU:HD22	1:A:767:ASN:HB3	2.00	0.43
1:A:432:GLN:NE2	1:A:445:TRP:HB2	2.31	0.43
1:A:601:GLU:O	1:A:605:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:LEU:O	1:A:710:ILE:N	2.50	0.43
1:A:345:ILE:HG13	1:A:345:ILE:O	2.19	0.43
1:A:567:ARG:HG3	1:A:599:VAL:HG23	2.00	0.43
1:A:198:MET:HG2	1:A:260:ALA:CB	2.48	0.43
1:A:341:GLU:HB2	1:A:345:ILE:HG22	2.01	0.43
1:A:611:PHE:O	1:A:614:PHE:HB2	2.19	0.43
1:A:692:ALA:HB1	1:A:702:ILE:HG13	1.98	0.43
1:A:702:ILE:H	1:A:702:ILE:CD1	2.31	0.43
1:A:614:PHE:CE1	1:A:622:ARG:HD2	2.53	0.43
1:A:333:GLU:HG3	4:A:890:HOH:O	2.17	0.43
1:A:177:TYR:HB2	1:A:200:ARG:HG3	2.01	0.43
1:A:649:ASP:HA	1:A:652:ARG:CB	2.49	0.43
1:A:574:MET:HE1	1:A:592:VAL:HG12	2.01	0.42
1:A:770:LEU:C	1:A:770:LEU:HD13	2.39	0.42
1:A:258:ASN:O	1:A:262:VAL:HG23	2.19	0.42
1:A:178:ARG:N	4:A:936:HOH:O	2.47	0.42
1:A:727:VAL:O	1:A:731:ILE:HG13	2.19	0.42
1:A:362:GLU:HG3	1:A:370:PHE:CG	2.54	0.42
1:A:706:LEU:HD13	1:A:713:VAL:CG2	2.43	0.42
1:A:428:ILE:O	1:A:467:SER:HA	2.19	0.42
1:A:453:LYS:HA	1:A:472:GLY:O	2.19	0.42
1:A:698:GLY:O	1:A:702:ILE:CD1	2.68	0.42
1:A:218:LYS:HZ3	1:A:220:HIS:CD2	2.38	0.42
1:A:674:MET:CG	1:A:679:GLU:HB2	2.48	0.42
1:A:253:VAL:HB	1:A:583:GLU:HG3	2.02	0.42
1:A:451:ILE:O	1:A:457:VAL:HA	2.20	0.42
1:A:269:HIS:HE1	1:A:287:ASN:O	2.02	0.42
1:A:269:HIS:CE1	1:A:291:ALA:HB2	2.55	0.42
1:A:735:GLY:HA2	1:A:740:ASP:CG	2.40	0.42
1:A:637:LYS:HA	1:A:640:LEU:HB2	2.01	0.42
1:A:642:LYS:O	1:A:646:VAL:HG12	2.19	0.42
1:A:631:LEU:HG	1:A:661:LYS:HB3	2.00	0.42
1:A:451:ILE:CD1	1:A:476:ILE:HG13	2.50	0.42
1:A:713:VAL:HA	1:A:716:TYR:CD2	2.54	0.42
1:A:14:ILE:HD13	1:A:128:ASP:OD1	2.19	0.42
1:A:99:HIS:CE1	1:A:101:GLU:HB2	2.55	0.42
1:A:705:ASN:HD21	1:A:709:ILE:HG21	1.80	0.41
1:A:707:ASP:OD1	1:A:743:ASP:OD1	2.37	0.41
1:A:218:LYS:NZ	1:A:220:HIS:CD2	2.78	0.41
1:A:214:TYR:OH	1:A:236:GLY:HA2	2.20	0.41
1:A:705:ASN:HD21	1:A:709:ILE:CD1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:N	1:A:195:PRO:HD2	2.35	0.41
1:A:31:ASP:HA	1:A:64:GLY:H	1.84	0.41
1:A:665:ASN:HA	1:A:701:PHE:CE2	2.55	0.41
1:A:117:TYR:CD1	1:A:117:TYR:N	2.88	0.41
1:A:732:PRO:HB2	1:A:767:ASN:HD21	1.85	0.41
1:A:3:VAL:HG11	1:A:6:TYR:CE2	2.55	0.41
1:A:473:LEU:HD23	1:A:474:ILE:C	2.41	0.41
1:A:705:ASN:OD1	1:A:709:ILE:HD12	2.21	0.41
1:A:726:THR:HG22	1:A:730:MET:CE	2.50	0.41
1:A:772:GLU:HA	1:A:772:GLU:OE2	2.21	0.41
1:A:703:PHE:HA	1:A:706:LEU:CB	2.36	0.41
1:A:702:ILE:C	1:A:704:ALA:H	2.24	0.41
1:A:740:ASP:O	1:A:743:ASP:HB2	2.20	0.41
1:A:656:ILE:HA	1:A:659:PHE:CD2	2.56	0.41
1:A:428:ILE:HD12	1:A:473:LEU:HD13	2.02	0.41
1:A:533:ILE:HD11	1:A:548:ILE:HD13	2.02	0.41
1:A:257:ARG:HD2	1:A:308:PHE:CZ	2.56	0.41
1:A:9:THR:HA	1:A:124:THR:O	2.21	0.41
1:A:11:ASP:HA	1:A:126:VAL:HB	2.03	0.41
1:A:402:PRO:O	1:A:406:VAL:HG23	2.21	0.41
1:A:409:TYR:CD2	1:A:446:PRO:HD2	2.56	0.41
1:A:706:LEU:HD12	1:A:710:ILE:HA	2.02	0.40
1:A:8:LEU:HD12	1:A:23:GLU:HB3	2.03	0.40
1:A:468:ILE:HD13	1:A:468:ILE:H	1.86	0.40
1:A:271:TRP:HA	1:A:275:LEU:HB2	2.03	0.40
1:A:714:ILE:N	1:A:714:ILE:HD12	2.36	0.40
1:A:655:ILE:HG22	1:A:659:PHE:CE1	2.56	0.40
1:A:558:LEU:CD2	1:A:767:ASN:HB3	2.50	0.40
1:A:108:MET:O	1:A:109:PHE:HB3	2.21	0.40
1:A:29:ALA:HB2	1:A:67:GLN:N	2.37	0.40
1:A:216:LEU:HB3	1:A:217:PRO:HD2	2.02	0.40
1:A:440:GLU:C	1:A:441:GLU:HG2	2.41	0.40
1:A:363:ASP:HA	4:A:947:HOH:O	2.21	0.40
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.86	0.40
1:A:248:ALA:C	1:A:250:ASN:H	2.24	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	778/780 (100%)	674 (87%)	82 (10%)	22 (3%)	6 15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	THR
1	A	635	ASP
1	A	702	ILE
1	A	102	ALA
1	A	464	ASP
1	A	778	ALA
1	A	101	GLU
1	A	648	ARG
1	A	678	THR
1	A	680	ILE
1	A	692	ALA
1	A	775	ARG
1	A	145	SER
1	A	347	ASP
1	A	674	MET
1	A	716	TYR
1	A	749	GLY
1	A	84	SER
1	A	693	LEU
1	A	80	SER
1	A	697	PRO
1	A	339	PRO

### 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	677/677 (100%)	632 (93%)	45 (7%)	21	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	93	ASN
1	A	130	ASP
1	A	184	LEU
1	A	187	LEU
1	A	198	MET
1	A	218	LYS
1	A	235	TRP
1	A	261	ASN
1	A	266	GLU
1	A	286	LEU
1	A	287	ASN
1	A	288	GLU
1	A	335	ASP
1	A	341	GLU
1	A	347	ASP
1	A	447	VAL
1	A	450	ASN
1	A	464	ASP
1	A	468	ILE
1	A	469	GLU
1	A	477	ASN
1	A	487	LEU
1	A	497	MET
1	A	531	GLN
1	A	555	LEU
1	A	558	LEU
1	A	581	GLN
1	A	583	GLU
1	A	596	TYR
1	A	624	SER
1	A	663	LYS
1	A	668	LEU
1	A	683	GLN
1	A	693	LEU

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Mol	Chain	Res	Type
1	A	700	GLU
1	A	703	PHE
1	A	709	ILE
1	A	712	LEU
1	A	717	PHE
1	A	718	THR
1	A	725	ARG
1	A	730	MET
1	A	736	LEU
1	A	764	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	47	ASN
1	A	58	GLN
1	A	69	GLN
1	A	114	HIS
1	A	136	ASN
1	A	153	GLN
1	A	220	HIS
1	A	234	ASN
1	A	261	ASN
1	A	287	ASN
1	A	328	ASN
1	A	432	GLN
1	A	438	ASN
1	A	477	ASN
1	A	523	HIS
1	A	531	GLN
1	A	551	GLN
1	A	683	GLN
1	A	705	ASN
1	A	747	ASN
1	A	767	ASN
1	A	776	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	A	801	-	4,4,4	0.43	0	6,6,6	0.11	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
3	SO4	A	801	-	-	0/0/0/0	0/0/0/0

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, 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	772/780 (98%)	0.15	60 (7%) 16 14	14, 40, 83, 103	20 (2%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	666	THR	8.3
1	A	741	ALA	7.3
1	A	780	LYS	7.0
1	A	345	ILE	6.6
1	A	708	ARG	6.1
1	A	777	THR	5.9
1	A	779	VAL	5.7
1	A	665	ASN	5.5
1	A	678	THR	5.4
1	A	745	VAL	5.0
1	A	455	ASP	5.0
1	A	674	MET	5.0
1	A	751	LYS	4.9
1	A	717	PHE	4.5
1	A	743	ASP	4.4
1	A	346	PHE	4.1
1	A	667	ASP	3.8
1	A	707	ASP	3.5
1	A	679	GLU	3.4
1	A	680	ILE	3.3
1	A	752	ASN	3.3
1	A	337	ARG	3.3
1	A	613	ASP	3.2
1	A	637	LYS	3.1
1	A	647	ASP	3.1
1	A	716	TYR	3.1
1	A	740	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	739	PRO	3.0
1	A	730	MET	2.8
1	A	755	MET	2.7
1	A	738	HIS	2.6
1	A	701	PHE	2.6
1	A	735	GLY	2.5
1	A	700	GLU	2.5
1	A	71	ILE	2.5
1	A	597	VAL	2.4
1	A	634	GLY	2.4
1	A	335	ASP	2.4
1	A	604	ALA	2.4
1	A	632	VAL	2.3
1	A	664	SER	2.3
1	A	633	THR	2.3
1	A	567	ARG	2.3
1	A	624	SER	2.2
1	A	640	LEU	2.2
1	A	581	GLN	2.2
1	A	648	ARG	2.2
1	A	616	SER	2.2
1	A	48	GLY	2.2
1	A	342	ILE	2.1
1	A	748	ILE	2.1
1	A	742	GLU	2.1
1	A	652	ARG	2.1
1	A	249	GLU	2.1
1	A	703	PHE	2.1
1	A	705	ASN	2.0
1	A	682	LYS	2.0
1	A	340	ASP	2.0
1	A	600	ASP	2.0
1	A	696	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	800	1/1	0.95	0.07	-2.37	35,35,35,35	0
3	SO4	A	801	5/5	0.94	0.19	-	54,56,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.