Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2024 – 08:48 AM EDT

PDB ID	:	4KKD
Title	:	The X-ray crystal structure of Mannose-binding lectin-associated serine proteinase-3 reveals the structural basis for enzyme inactivity associated with the 3MC syndrome
Authors	:	Yongqing, T.; Wilmann, P.G.; Reeve, S.B.; Coetzer, T.H.; Smith, A.I.; Whisstock, J.C.; Pike, R.N.; Wijeyewickrema, L.C.
Deposited on	:	2013-05-05
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

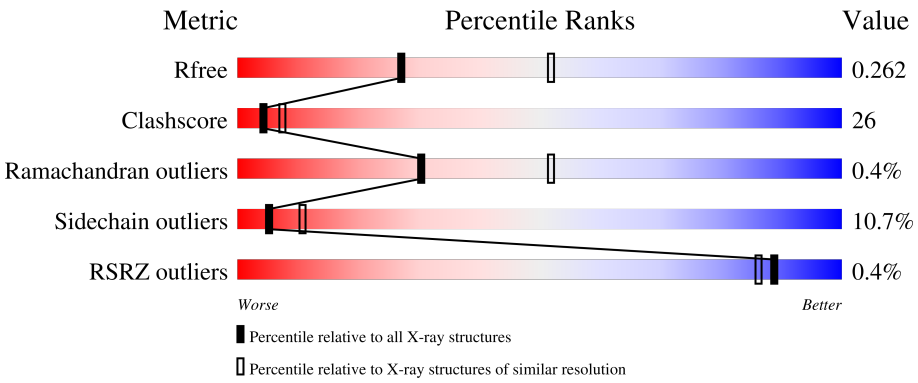
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	433	50% 35% 5% 10%
1	B	433	54% 36% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IMD	B	801	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6408 atoms, of which 5 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.

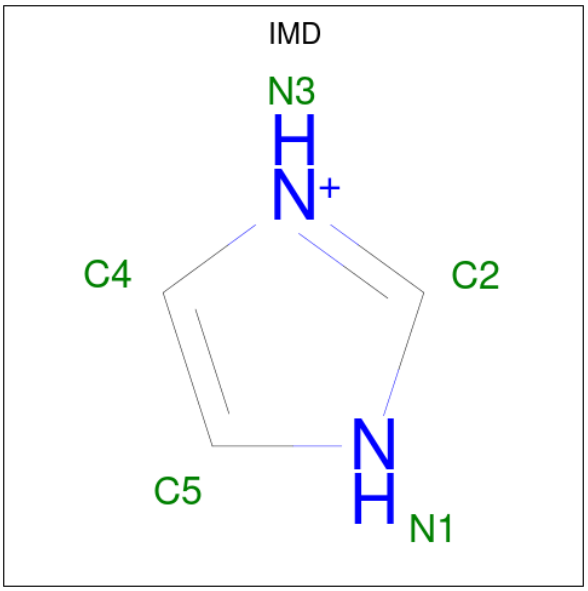
- Molecule 1 is a protein called Mannan-binding lectin serine protease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3049	1938	515	575	21	0	0	0
1	B	405	3148	2001	533	593	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	MET	-	expression tag	UNP P48740
A	297	ALA	-	expression tag	UNP P48740
A	448	GLN	LYS	engineered mutation	UNP P48740
A	666	GLU	GLY	variant	UNP P48740
B	296	MET	-	expression tag	UNP P48740
B	297	ALA	-	expression tag	UNP P48740
B	448	GLN	LYS	engineered mutation	UNP P48740
B	666	GLU	GLY	variant	UNP P48740

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
2	B	1	10	3	5	2	0	0

- Molecule 3 is water.

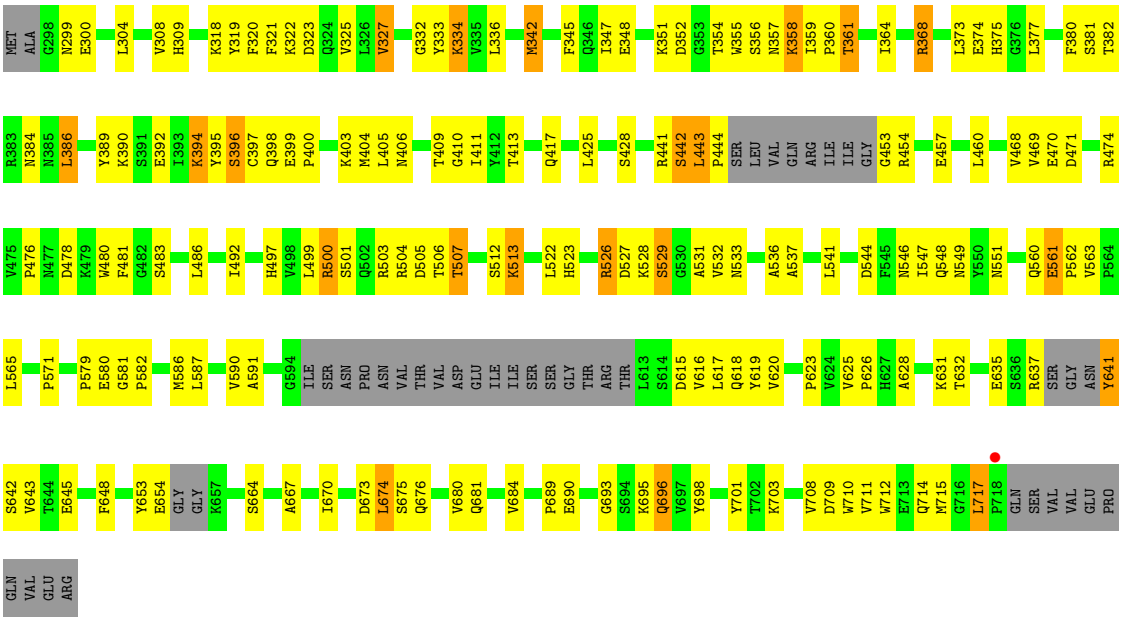
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	100	100	100	0	0
			Total	O		
3	B	101	101	101	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

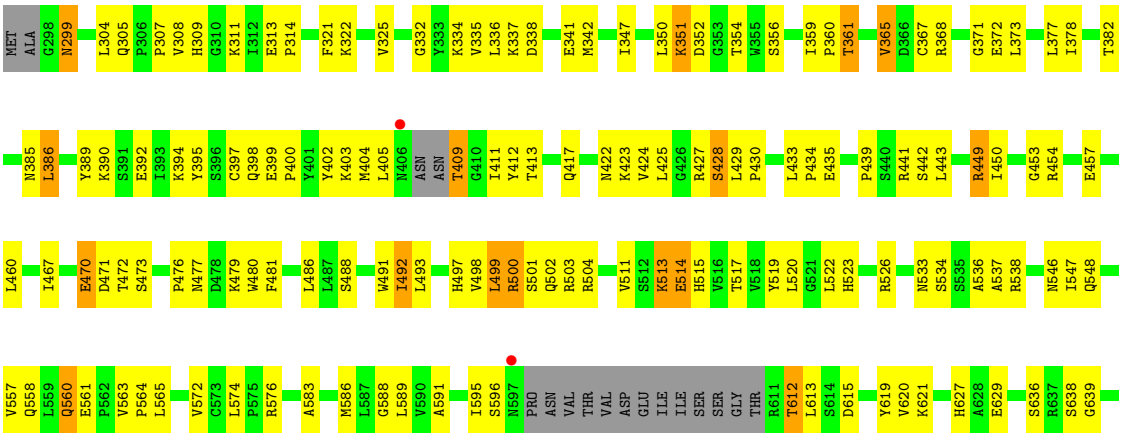
• Molecule 1: Mannan-binding lectin serine protease 1

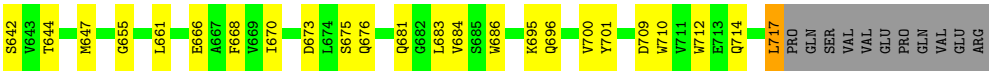
Chain A: 50% 35% 5% 10%



• Molecule 1: Mannan-binding lectin serine protease 1

Chain B: 54% 36% • 6%




S642
V643
T644
M647
G655
L661
E666
A667
F668
V669
I670
D673
L674
S675
Q676
Q681
G682
L683
V684
S685
W686
K695
Q696
V700
Y701
D709
W710
V711
W712
E713
Q714
L717
PRO
GLN
SER
VAL
VAL
GLU
PRO
GLN
VAL
GLU
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	72.84Å 292.92Å 43.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 2.60 48.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.82-2.60) 99.9 (48.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.194 , 0.260 0.198 , 0.262	Depositor DCC
R_{free} test set	1034 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6408	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: IMD

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	0.45	0/3129	0.59	0/4263
1	B	0.46	0/3229	0.62	0/4398
All	All	0.46	0/6358	0.60	0/8661

There are no bond length outliers.

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	3049	0	2942	177	0
1	B	3148	0	3059	153	0
2	B	5	5	5	9	0
3	A	100	0	0	9	0
3	B	101	0	0	17	0
All	All	6403	5	6006	323	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 26.

All (323) 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:670:ILE:HD12	1:A:681:GLN:HG3	1.26	1.16
1:A:674:LEU:HD23	1:A:674:LEU:H	1.03	1.11
1:B:394:LYS:HE2	1:B:411:ILE:HD11	1.31	1.07
1:A:641:TYR:N	3:A:884:HOH:O	1.86	1.05
1:A:637:ARG:HB2	1:A:637:ARG:HH11	1.17	1.02
1:A:382:THR:HG22	1:A:384:ASN:H	1.21	1.01
1:B:520:LEU:HD12	1:B:563:VAL:HG11	1.40	1.00
1:A:674:LEU:HD23	1:A:674:LEU:N	1.78	0.99
1:A:546:ASN:ND2	1:A:549:ASN:OD1	1.97	0.96
1:B:439:PRO:HG2	2:B:801:IMD:H2	1.47	0.94
1:A:674:LEU:H	1:A:674:LEU:CD2	1.81	0.93
1:B:443:LEU:HG	2:B:801:IMD:H4	1.50	0.93
1:B:620:VAL:HG23	1:B:661:LEU:HD11	1.51	0.92
1:A:637:ARG:HB2	1:A:637:ARG:NH1	1.84	0.92
1:B:572:VAL:O	3:B:934:HOH:O	1.89	0.91
1:A:712:TRP:CE3	1:A:717:LEU:HD23	2.09	0.88
1:A:504:ARG:HH22	1:B:500:ARG:HD3	1.37	0.88
1:A:670:ILE:HD12	1:A:681:GLN:CG	2.03	0.87
1:B:439:PRO:CG	2:B:801:IMD:H2	2.04	0.87
1:B:499:LEU:O	1:B:511:VAL:HG23	1.75	0.87
1:A:544:ASP:OD1	3:A:893:HOH:O	1.91	0.87
1:A:579:PRO:O	1:A:703:LYS:NZ	2.09	0.86
1:A:637:ARG:NH2	1:A:641:TYR:HA	1.91	0.85
1:A:673:ASP:O	1:A:676:GLN:NE2	2.09	0.85
1:A:470:GLU:OE2	3:A:886:HOH:O	1.95	0.84
1:A:453:GLY:HA2	1:A:620:VAL:HG12	1.60	0.82
1:A:380:PHE:O	3:A:827:HOH:O	1.97	0.81
1:B:595:ILE:O	1:B:596:SER:HB3	1.80	0.81
1:B:583:ALA:H	1:B:586:MET:HE3	1.45	0.81
1:A:345:PHE:HE2	1:A:347:ILE:HD11	1.44	0.80
1:B:405:LEU:HD13	1:B:433:LEU:HD12	1.63	0.79
1:B:583:ALA:H	1:B:586:MET:CE	1.95	0.79
1:A:442:SER:O	1:A:444:PRO:HD3	1.82	0.78
1:B:500:ARG:NH2	1:B:547:ILE:HD13	1.99	0.78
1:B:394:LYS:HE2	1:B:411:ILE:CD1	2.11	0.78
1:B:612:THR:HG22	1:B:613:LEU:H	1.47	0.78
1:A:347:ILE:CD1	1:A:357:ASN:HB2	2.14	0.77
1:A:417:GLN:N	1:A:417:GLN:OE1	2.16	0.77
1:A:476:PRO:O	1:B:503:ARG:NH2	2.19	0.76
1:B:502:GLN:OE1	1:B:502:GLN:N	2.13	0.76
1:A:382:THR:HG22	1:A:384:ASN:N	2.01	0.75
1:A:711:VAL:HG12	1:A:715:MET:HE2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:CYS:SG	1:A:404:MET:HG3	2.27	0.74
1:A:345:PHE:CE2	1:A:347:ILE:HD11	2.22	0.74
1:B:460:LEU:O	2:B:801:IMD:N1	2.19	0.74
1:A:637:ARG:HH22	1:A:641:TYR:HA	1.49	0.73
1:B:620:VAL:HG23	1:B:661:LEU:CD1	2.18	0.73
1:B:533:ASN:ND2	3:B:991:HOH:O	2.22	0.72
1:A:712:TRP:HE3	1:A:717:LEU:HD23	1.52	0.72
1:A:342:MET:HE2	1:A:345:PHE:HB2	1.72	0.72
1:B:321:PHE:O	1:B:322:LYS:HB2	1.89	0.72
1:B:439:PRO:HG2	2:B:801:IMD:C2	2.20	0.71
1:A:670:ILE:CD1	1:A:681:GLN:HG3	2.13	0.71
1:B:299:ASN:OD1	1:B:299:ASN:N	2.21	0.71
1:A:300:GLU:HB2	1:A:320:PHE:CE1	2.26	0.71
1:B:338:ASP:O	3:B:1000:HOH:O	2.09	0.71
1:B:449:ARG:NH1	1:B:454:ARG:HD3	2.06	0.71
1:B:583:ALA:N	1:B:586:MET:HE3	2.05	0.71
1:B:684:VAL:HG22	1:B:701:TYR:CE2	2.26	0.70
1:A:506:THR:HG22	1:A:548:GLN:OE1	1.92	0.70
1:A:500:ARG:CD	1:A:547:ILE:HD13	2.22	0.70
1:A:637:ARG:HH11	1:A:637:ARG:CB	2.02	0.70
1:A:342:MET:HE1	1:A:345:PHE:HD1	1.57	0.69
1:B:629:GLU:OE2	1:B:696:GLN:NE2	2.26	0.69
1:B:449:ARG:CZ	1:B:454:ARG:HD3	2.22	0.68
1:B:443:LEU:CG	2:B:801:IMD:H4	2.23	0.68
1:B:655:GLY:O	3:B:969:HOH:O	2.12	0.68
1:B:443:LEU:HG	2:B:801:IMD:C4	2.24	0.68
1:B:325:VAL:HG22	1:B:347:ILE:HG12	1.75	0.68
1:A:500:ARG:HD2	1:A:547:ILE:HD13	1.76	0.68
1:B:493:LEU:HD11	1:B:683:LEU:HD11	1.75	0.68
1:A:527:ASP:OD1	1:A:529:SER:HB3	1.93	0.67
1:A:321:PHE:CD1	1:A:351:LYS:HA	2.30	0.67
1:A:711:VAL:HG12	1:A:715:MET:CE	2.25	0.66
1:B:443:LEU:HD11	1:B:589:LEU:HD11	1.76	0.66
1:A:505:ASP:OD1	1:A:507:THR:HG23	1.95	0.66
1:A:358:LYS:O	3:A:828:HOH:O	2.13	0.66
1:A:389:TYR:CE2	1:A:390:LYS:HE3	2.30	0.66
1:B:514:GLU:OE1	3:B:972:HOH:O	2.13	0.66
1:A:712:TRP:CZ3	1:A:717:LEU:HD23	2.31	0.66
1:A:684:VAL:HG23	1:A:701:TYR:CE2	2.31	0.66
1:A:637:ARG:HH21	1:A:641:TYR:HB3	1.60	0.66
1:A:528:LYS:O	1:A:531:ALA:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LYS:HG2	1:B:411:ILE:HD13	1.78	0.65
1:B:513:LYS:HD3	1:B:536:ALA:O	1.96	0.65
1:B:372:GLU:HG3	1:B:373:LEU:N	2.11	0.65
1:A:382:THR:CG2	1:A:384:ASN:H	2.05	0.64
1:B:382:THR:CG2	1:B:386:LEU:H	2.10	0.64
1:B:409:THR:O	3:B:981:HOH:O	2.14	0.64
1:B:336:LEU:HB3	1:B:361:THR:HG22	1.79	0.64
1:A:675:SER:O	1:A:676:GLN:HB2	1.97	0.64
1:B:453:GLY:HA2	1:B:620:VAL:HG22	1.80	0.64
1:A:300:GLU:HB2	1:A:320:PHE:CD1	2.33	0.63
1:A:582:PRO:N	3:A:879:HOH:O	2.30	0.63
1:B:520:LEU:CD1	1:B:563:VAL:HG11	2.22	0.62
1:B:695:LYS:HG2	1:B:696:GLN:HG3	1.80	0.62
1:B:304:LEU:HD22	1:B:359:ILE:HD11	1.81	0.62
1:B:382:THR:HG23	1:B:385:ASN:H	1.65	0.62
1:B:500:ARG:CZ	1:B:547:ILE:HD13	2.29	0.61
1:B:382:THR:HG21	1:B:386:LEU:H	1.66	0.61
1:A:308:VAL:O	1:A:309:HIS:HB2	2.00	0.60
1:A:637:ARG:NH2	1:A:641:TYR:CA	2.64	0.60
1:A:637:ARG:NH2	1:A:641:TYR:HB3	2.16	0.60
1:A:505:ASP:CG	1:A:507:THR:HG23	2.23	0.59
1:A:425:LEU:HB3	1:A:428:SER:O	2.02	0.59
1:B:307:PRO:HD3	1:B:359:ILE:CG2	2.33	0.59
1:A:394:LYS:HA	1:A:410:GLY:O	2.03	0.59
1:B:332:GLY:O	1:B:365:VAL:HG13	2.03	0.59
1:B:352:ASP:O	3:B:910:HOH:O	2.16	0.59
1:B:546:ASN:OD1	1:B:548:GLN:N	2.36	0.59
1:A:673:ASP:HB3	1:A:674:LEU:HD23	1.84	0.59
1:A:582:PRO:HB3	1:A:586:MET:CE	2.33	0.59
1:A:347:ILE:HG22	1:A:355:TRP:CE3	2.38	0.58
1:A:674:LEU:HG	1:A:675:SER:H	1.68	0.58
1:B:519:TYR:O	1:B:520:LEU:HD23	2.04	0.58
1:A:643:VAL:O	1:A:643:VAL:CG2	2.50	0.58
1:A:546:ASN:ND2	1:A:549:ASN:H	2.02	0.58
1:A:500:ARG:HG2	1:A:500:ARG:HH11	1.68	0.57
1:A:377:LEU:HD23	1:A:396:SER:O	2.03	0.57
1:B:441:ARG:NH1	1:B:457:GLU:OE1	2.37	0.57
1:B:502:GLN:O	1:B:502:GLN:HG2	2.03	0.57
1:B:666:GLU:O	1:B:684:VAL:HG23	2.04	0.57
1:B:382:THR:HG23	1:B:385:ASN:N	2.19	0.57
1:B:405:LEU:HD13	1:B:433:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HB	1:B:342:MET:O	2.04	0.57
1:B:498:VAL:HG12	1:B:499:LEU:HD13	1.87	0.57
1:B:486:LEU:HG	1:B:488:SER:O	2.05	0.57
1:A:453:GLY:HA2	1:A:620:VAL:CG1	2.32	0.57
1:A:684:VAL:CG2	1:A:701:TYR:CE2	2.88	0.57
1:B:546:ASN:OD1	1:B:548:GLN:HB2	2.05	0.56
1:A:474:ARG:NH2	1:B:502:GLN:O	2.39	0.56
1:A:503:ARG:HA	1:B:502:GLN:HG3	1.87	0.56
1:B:400:PRO:O	1:B:435:GLU:HG3	2.05	0.56
1:B:399:GLU:HG2	1:B:403:LYS:HE2	1.88	0.56
1:A:689:PRO:HD2	1:A:690:GLU:OE1	2.05	0.56
1:A:377:LEU:HD23	1:A:377:LEU:H	1.71	0.56
1:A:497:HIS:O	1:B:504:ARG:NH2	2.38	0.56
1:B:434:PRO:HB3	1:B:565:LEU:CD2	2.36	0.56
1:B:321:PHE:CZ	1:B:322:LYS:HE2	2.41	0.55
1:A:381:SER:OG	1:A:392:GLU:HG2	2.07	0.55
1:B:449:ARG:HG3	1:B:449:ARG:HH11	1.71	0.55
1:B:352:ASP:OD1	1:B:354:THR:HG23	2.06	0.55
1:B:453:GLY:CA	1:B:620:VAL:HG22	2.37	0.55
1:A:632:THR:HA	1:A:635:GLU:CG	2.36	0.55
1:A:321:PHE:CE2	1:A:322:LYS:HG3	2.42	0.55
1:A:582:PRO:HB3	1:A:586:MET:HE2	1.88	0.55
1:B:443:LEU:HD11	1:B:589:LEU:CD1	2.36	0.55
1:B:454:ARG:HG3	3:B:936:HOH:O	2.06	0.55
1:B:389:TYR:O	1:B:390:LYS:HB2	2.07	0.54
1:A:399:GLU:CB	1:A:400:PRO:HA	2.36	0.54
1:A:503:ARG:NH1	1:A:505:ASP:OD2	2.40	0.54
1:B:564:PRO:HG2	3:B:958:HOH:O	2.07	0.54
1:B:308:VAL:HG12	1:B:309:HIS:ND1	2.22	0.54
1:B:337:LYS:O	1:B:338:ASP:HB2	2.08	0.54
1:B:425:LEU:HD22	1:B:428:SER:HB3	1.90	0.54
1:B:537:ALA:HB2	1:B:560:GLN:HA	1.90	0.54
1:A:300:GLU:HG3	1:A:319:TYR:O	2.08	0.54
1:A:399:GLU:HB3	1:A:400:PRO:HA	1.89	0.54
1:A:565:LEU:HD23	1:A:565:LEU:N	2.22	0.54
1:A:581:GLY:HA2	1:A:703:LYS:HD2	1.89	0.53
1:A:384:ASN:HB3	1:A:386:LEU:HD13	1.90	0.53
1:B:424:VAL:HG12	1:B:425:LEU:N	2.22	0.53
1:A:696:GLN:HG3	1:A:698:TYR:OH	2.09	0.53
1:A:411:ILE:O	3:A:809:HOH:O	2.19	0.52
1:A:375:HIS:O	1:A:398:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ARG:NH1	1:A:501:SER:O	2.42	0.52
1:A:581:GLY:C	3:A:879:HOH:O	2.47	0.52
1:A:500:ARG:HD2	1:A:547:ILE:CD1	2.39	0.52
1:A:325:VAL:HG23	1:A:347:ILE:HB	1.92	0.52
1:A:591:ALA:HA	1:A:618:GLN:O	2.10	0.51
1:A:336:LEU:HB3	1:A:361:THR:HG22	1.91	0.51
1:A:377:LEU:HD21	1:A:396:SER:OG	2.10	0.51
1:B:402:TYR:HE1	3:B:961:HOH:O	1.93	0.51
1:A:323:ASP:O	1:A:348:GLU:HA	2.10	0.51
1:A:486:LEU:HB3	1:A:571:PRO:HA	1.93	0.51
1:B:588:GLY:HA3	1:B:668:PHE:CE1	2.46	0.51
1:A:513:LYS:HG3	1:A:536:ALA:O	2.11	0.51
1:A:377:LEU:HD23	1:A:377:LEU:N	2.26	0.51
1:A:684:VAL:HG23	1:A:701:TYR:HE2	1.73	0.51
1:B:612:THR:HG22	1:B:613:LEU:N	2.23	0.51
1:A:333:TYR:C	1:A:334:LYS:HD2	2.32	0.50
1:A:395:TYR:N	1:A:410:GLY:O	2.35	0.50
1:A:625:VAL:HG13	1:A:626:PRO:HD2	1.93	0.50
1:B:321:PHE:O	1:B:322:LYS:CB	2.59	0.50
1:B:644:THR:OG1	1:B:647:MET:HG3	2.12	0.50
1:A:526:ARG:HD2	1:A:615:ASP:OD2	2.11	0.50
1:A:327:VAL:HG13	1:A:345:PHE:HB3	1.93	0.49
1:A:643:VAL:O	1:A:643:VAL:HG22	2.11	0.49
1:A:648:PHE:HD2	1:A:703:LYS:HG3	1.78	0.49
1:B:591:ALA:HA	1:B:619:TYR:HA	1.93	0.49
1:A:632:THR:HA	1:A:635:GLU:HG3	1.94	0.49
1:A:325:VAL:CG2	1:A:347:ILE:HB	2.43	0.48
1:B:311:LYS:HE2	3:B:951:HOH:O	2.13	0.48
1:B:332:GLY:C	1:B:365:VAL:HG13	2.34	0.48
1:B:373:LEU:HD11	1:B:430:PRO:O	2.13	0.48
1:A:546:ASN:HD21	1:A:548:GLN:HB2	1.79	0.48
1:B:367:CYS:C	1:B:368:ARG:HG3	2.34	0.48
1:A:354:THR:HG22	1:A:355:TRP:O	2.14	0.48
1:B:472:THR:HG22	1:B:477:ASN:OD1	2.13	0.48
1:B:378:ILE:HG12	1:B:395:TYR:CE1	2.49	0.47
1:A:332:GLY:HA3	1:A:389:TYR:CD2	2.50	0.47
1:A:304:LEU:HD21	1:A:355:TRP:CE2	2.50	0.47
1:A:631:LYS:O	1:A:635:GLU:HG2	2.14	0.47
1:B:392:GLU:HG3	1:B:413:THR:OG1	2.14	0.47
1:B:441:ARG:HG2	1:B:442:SER:N	2.29	0.47
1:A:300:GLU:CD	1:A:318:LYS:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:GLU:HG3	1:A:695:LYS:HA	1.96	0.47
1:B:627:HIS:NE2	1:B:644:THR:O	2.47	0.47
1:A:632:THR:HA	1:A:635:GLU:HG2	1.97	0.47
1:B:411:ILE:O	1:B:422:ASN:ND2	2.46	0.47
1:B:443:LEU:HD21	2:B:801:IMD:H5	1.95	0.47
1:A:409:THR:O	3:A:883:HOH:O	2.20	0.47
1:B:402:TYR:O	1:B:403:LYS:HD2	2.15	0.47
1:B:710:TRP:O	1:B:714:GLN:HG2	2.15	0.47
1:A:505:ASP:CG	1:A:507:THR:CG2	2.83	0.47
1:B:427:ARG:O	3:B:955:HOH:O	2.20	0.47
1:B:686:TRP:CH2	1:B:700:VAL:HG21	2.50	0.47
1:B:449:ARG:HD2	1:B:449:ARG:HA	1.76	0.47
1:B:472:THR:HA	1:B:477:ASN:OD1	2.15	0.46
1:B:596:SER:HB2	1:B:613:LEU:HD21	1.96	0.46
1:B:497:HIS:HA	1:B:500:ARG:HG3	1.97	0.46
1:B:620:VAL:HG12	1:B:621:LYS:O	2.16	0.46
1:B:350:LEU:HD11	1:B:356:SER:HA	1.97	0.46
1:A:504:ARG:HD2	1:B:480:TRP:CD2	2.51	0.46
1:A:394:LYS:HG3	1:A:411:ILE:HD13	1.98	0.46
1:A:628:ALA:O	1:A:632:THR:HG23	2.16	0.46
1:A:321:PHE:CE2	1:A:322:LYS:HE2	2.51	0.45
1:A:347:ILE:HG22	1:A:355:TRP:HE3	1.79	0.45
1:A:561:GLU:OE2	1:A:561:GLU:HA	2.16	0.45
1:B:574:LEU:HD12	1:B:712:TRP:CH2	2.50	0.45
1:A:631:LYS:HB2	1:A:643:VAL:HG22	1.98	0.45
1:B:394:LYS:HG2	1:B:411:ILE:CD1	2.45	0.45
1:A:342:MET:HE1	1:A:345:PHE:CD1	2.44	0.45
1:A:547:ILE:HG13	1:A:547:ILE:O	2.17	0.45
1:A:351:LYS:HG3	1:A:352:ASP:N	2.32	0.45
1:A:443:LEU:HD13	1:A:443:LEU:HA	1.53	0.45
1:B:389:TYR:CE2	1:B:390:LYS:HD2	2.51	0.45
1:A:345:PHE:CE2	1:A:347:ILE:CD1	2.97	0.45
1:B:351:LYS:HE3	1:B:351:LYS:HB3	1.79	0.45
1:B:409:THR:CB	3:B:981:HOH:O	2.65	0.44
1:A:347:ILE:HD11	1:A:357:ASN:HB2	1.96	0.44
1:B:449:ARG:NH2	1:B:454:ARG:HD3	2.31	0.44
1:B:709:ASP:OD1	1:B:710:TRP:N	2.49	0.44
1:A:637:ARG:NH2	1:A:641:TYR:CB	2.80	0.44
1:A:443:LEU:CD1	1:A:444:PRO:HD2	2.48	0.44
1:A:503:ARG:NH2	1:B:476:PRO:O	2.50	0.44
1:B:307:PRO:HD3	1:B:359:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ARG:HB3	1:B:558:GLN:HB3	2.00	0.44
1:A:417:GLN:N	1:A:417:GLN:CD	2.71	0.44
1:A:710:TRP:O	1:A:714:GLN:HG2	2.18	0.44
1:B:371:GLY:N	3:B:960:HOH:O	2.06	0.44
1:A:333:TYR:CD2	1:A:364:ILE:HA	2.53	0.44
1:A:333:TYR:O	1:A:334:LYS:HD2	2.18	0.44
1:A:684:VAL:O	1:A:684:VAL:HG12	2.18	0.44
1:B:412:TYR:OH	1:B:428:SER:O	2.26	0.44
1:A:321:PHE:O	1:A:322:LYS:HB2	2.18	0.44
1:B:325:VAL:HG22	1:B:347:ILE:CG1	2.47	0.44
1:A:632:THR:O	1:A:635:GLU:HB2	2.18	0.43
1:B:454:ARG:HG2	1:B:454:ARG:HH11	1.83	0.43
1:B:313:GLU:HA	1:B:314:PRO:HA	1.69	0.43
1:A:373:LEU:HD12	1:A:374:GLU:H	1.83	0.43
1:A:499:LEU:HB2	1:A:541:LEU:HD21	2.00	0.43
1:A:468:VAL:HG22	1:A:481:PHE:CD2	2.53	0.43
1:A:590:VAL:O	1:A:619:TYR:HA	2.18	0.43
1:B:325:VAL:CG2	1:B:347:ILE:HG12	2.45	0.43
1:B:479:LYS:HE2	1:B:479:LYS:HB3	1.77	0.43
1:A:300:GLU:OE1	1:A:318:LYS:HD3	2.19	0.43
1:A:537:ALA:HB2	1:A:560:GLN:HA	2.00	0.43
1:A:703:LYS:HB3	1:A:703:LYS:HE2	1.86	0.43
1:A:673:ASP:HB3	1:A:674:LEU:H	1.69	0.43
1:B:394:LYS:CE	1:B:411:ILE:HD11	2.22	0.43
1:B:502:GLN:H	1:B:502:GLN:CD	2.08	0.43
1:B:675:SER:O	1:B:676:GLN:HB2	2.19	0.42
1:A:321:PHE:CD2	1:A:322:LYS:HE2	2.55	0.42
1:B:638:SER:HA	1:B:639:GLY:HA2	1.57	0.42
1:A:654:GLU:HA	1:A:693:GLY:O	2.20	0.42
1:A:377:LEU:N	1:A:377:LEU:CD2	2.83	0.42
1:A:503:ARG:HG3	1:A:505:ASP:OD1	2.19	0.42
1:B:397:CYS:SG	1:B:404:MET:HG3	2.60	0.42
1:A:409:THR:HB	1:A:411:ILE:HG12	2.02	0.42
1:A:532:VAL:HG11	1:A:563:VAL:HG12	2.01	0.42
1:A:561:GLU:HA	1:A:562:PRO:HD3	1.87	0.42
1:B:670:ILE:HD12	1:B:681:GLN:HG3	2.01	0.42
1:A:641:TYR:HB2	1:A:642:SER:H	1.65	0.42
1:B:409:THR:HB	3:B:981:HOH:O	2.20	0.42
1:B:467:ILE:O	1:B:481:PHE:HA	2.20	0.42
1:B:471:ASP:HA	1:B:515:HIS:CD2	2.54	0.42
1:B:491:TRP:CH2	1:B:558:GLN:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:LEU:HD12	1:A:717:LEU:HA	1.67	0.42
1:B:405:LEU:HD12	1:B:405:LEU:HA	1.83	0.41
1:B:351:LYS:HB2	3:B:916:HOH:O	2.20	0.41
1:B:638:SER:HA	3:B:964:HOH:O	2.20	0.41
1:B:443:LEU:CD1	2:B:801:IMD:H4	2.49	0.41
1:A:469:VAL:HG11	1:A:480:TRP:CZ2	2.56	0.41
1:B:499:LEU:C	1:B:511:VAL:HG23	2.39	0.41
1:B:526:ARG:HD3	1:B:615:ASP:OD2	2.21	0.41
1:A:321:PHE:CZ	1:A:322:LYS:HG3	2.55	0.41
1:A:347:ILE:HD12	1:A:357:ASN:HB2	1.99	0.41
1:A:389:TYR:O	1:A:390:LYS:HB2	2.20	0.41
1:A:581:GLY:O	1:A:582:PRO:C	2.58	0.41
1:A:711:VAL:CG1	1:A:715:MET:HE2	2.43	0.41
1:B:403:LYS:HD2	1:B:403:LYS:HA	1.82	0.41
1:B:434:PRO:HB3	1:B:565:LEU:HD21	2.02	0.41
1:A:334:LYS:HD2	1:A:334:LYS:N	2.35	0.41
1:A:708:VAL:HG23	1:A:709:ASP:N	2.36	0.41
1:B:449:ARG:NH1	1:B:449:ARG:HG3	2.33	0.41
1:B:491:TRP:CZ3	1:B:558:GLN:HB2	2.55	0.41
1:A:471:ASP:HB3	1:A:478:ASP:HB3	2.02	0.41
1:A:587:LEU:HD23	1:A:623:PRO:HA	2.03	0.41
1:B:492:ILE:CG1	1:B:557:VAL:HB	2.51	0.41
1:A:443:LEU:HD13	1:A:444:PRO:HD2	2.02	0.41
1:A:503:ARG:HH11	1:A:505:ASP:CG	2.22	0.41
1:B:686:TRP:CZ2	1:B:700:VAL:HG21	2.55	0.41
1:A:486:LEU:HD12	1:A:492:ILE:HD12	2.03	0.40
1:A:616:VAL:HG12	1:A:617:LEU:N	2.36	0.40
1:B:335:VAL:O	1:B:341:GLU:HA	2.20	0.40
1:B:470:GLU:HG3	1:B:479:LYS:HE2	2.02	0.40
1:A:528:LYS:O	1:A:531:ALA:CB	2.67	0.40
1:B:717:LEU:HD12	1:B:717:LEU:HA	1.76	0.40
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.88	0.40
1:A:441:ARG:HH12	1:A:457:GLU:HB3	1.87	0.40
1:A:457:GLU:H	1:A:460:LEU:HD12	1.86	0.40
1:A:667:ALA:HB1	1:A:680:VAL:HG23	2.03	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	380/433 (88%)	352 (93%)	26 (7%)	2 (0%)	25 47
1	B	399/433 (92%)	369 (92%)	29 (7%)	1 (0%)	37 59
All	All	779/866 (90%)	721 (93%)	55 (7%)	3 (0%)	30 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	B	360	PRO
1	A	360	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	340/379 (90%)	302 (89%)	38 (11%)	5 9
1	B	350/379 (92%)	314 (90%)	36 (10%)	6 12
All	All	690/758 (91%)	616 (89%)	74 (11%)	5 11

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	327	VAL
1	A	334	LYS

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Mol	Chain	Res	Type
1	A	342	MET
1	A	356	SER
1	A	358	LYS
1	A	359	ILE
1	A	361	THR
1	A	368	ARG
1	A	386	LEU
1	A	394	LYS
1	A	396	SER
1	A	403	LYS
1	A	406	ASN
1	A	413	THR
1	A	442	SER
1	A	443	LEU
1	A	454	ARG
1	A	483	SER
1	A	500	ARG
1	A	507	THR
1	A	512	SER
1	A	513	LYS
1	A	522	LEU
1	A	523	HIS
1	A	526	ARG
1	A	529	SER
1	A	533	ASN
1	A	551	ASN
1	A	561	GLU
1	A	580	GLU
1	A	641	TYR
1	A	645	GLU
1	A	653	TYR
1	A	664	SER
1	A	674	LEU
1	A	696	GLN
1	A	717	LEU
1	B	299	ASN
1	B	305	GLN
1	B	334	LYS
1	B	351	LYS
1	B	361	THR
1	B	365	VAL
1	B	377	LEU

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Mol	Chain	Res	Type
1	B	386	LEU
1	B	398	GLN
1	B	409	THR
1	B	417	GLN
1	B	423	LYS
1	B	428	SER
1	B	429	LEU
1	B	449	ARG
1	B	450	ILE
1	B	470	GLU
1	B	473	SER
1	B	492	ILE
1	B	499	LEU
1	B	500	ARG
1	B	501	SER
1	B	513	LYS
1	B	514	GLU
1	B	517	THR
1	B	522	LEU
1	B	523	HIS
1	B	534	SER
1	B	560	GLN
1	B	561	GLU
1	B	576	ARG
1	B	612	THR
1	B	636	SER
1	B	642	SER
1	B	673	ASP
1	B	717	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	IMD	B	801	-	3,5,5	0.68	0	4,5,5	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	B	801	-	-	-	0/1/1/1

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.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	IMD	9	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	390/433 (90%)	-0.36	1 (0%)	90	88	2, 17, 46, 66	0
1	B	405/433 (93%)	-0.49	2 (0%)	87	84	2, 15, 35, 59	0
All	All	795/866 (91%)	-0.43	3 (0%)	89	86	2, 16, 41, 66	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	718	PRO	2.6
1	B	406	ASN	2.3
1	B	597	ASN	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	IMD	B	801	5/5	0.92	0.12	11,18,22,23	0

6.5 Other polymers (i)

There are no such residues in this entry.