Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 09:25 PM EDT

PDB ID	:	3V65
Title	:	Crystal structure of agrin and LRP4 complex
Authors	:	Zong, Y.; Jin, R.
Deposited on	:	2011-12-18
Resolution	:	3.30 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 (1)) were used in the production of this report:

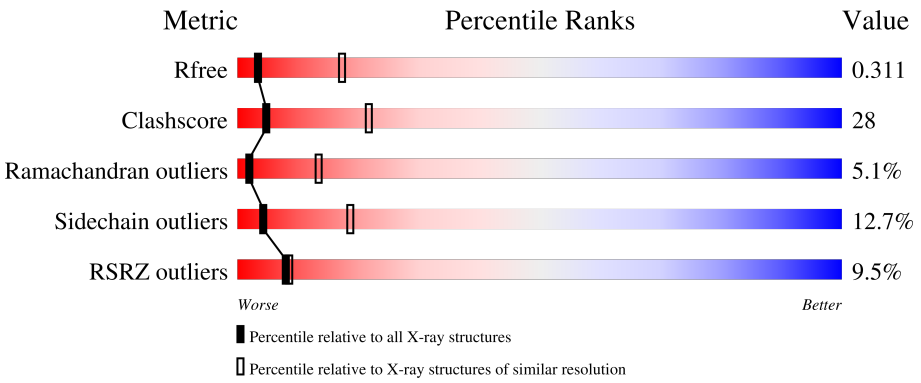
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	191	10%; 58%; 36%; 6%
1	C	191	19%; 46%; 42%; 10%; •
2	B	386	5%; 39%; 41%; 5%; •; 15%
2	D	386	7%; 44%; 41%; 13%; •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8566 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 Agrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1470	927	263	277	3	0	0	0
1	C	191	1470	927	263	277	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1758	ALA	-	EXPRESSION TAG	UNP P25304
C	1758	ALA	-	EXPRESSION TAG	UNP P25304

- Molecule 2 is a protein called Low-density lipoprotein receptor-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	330	2639	1657	489	478	15	0	0	0
2	D	377	2985	1854	557	551	23	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	738	GLN	-	EXPRESSION TAG	UNP Q9QYP1
D	738	GLN	-	EXPRESSION TAG	UNP Q9QYP1

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

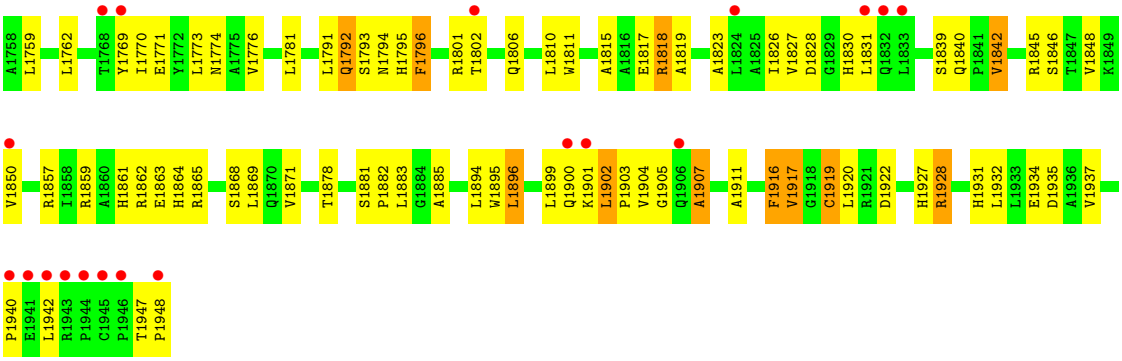
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
3	C	1	1	1	0	0

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.

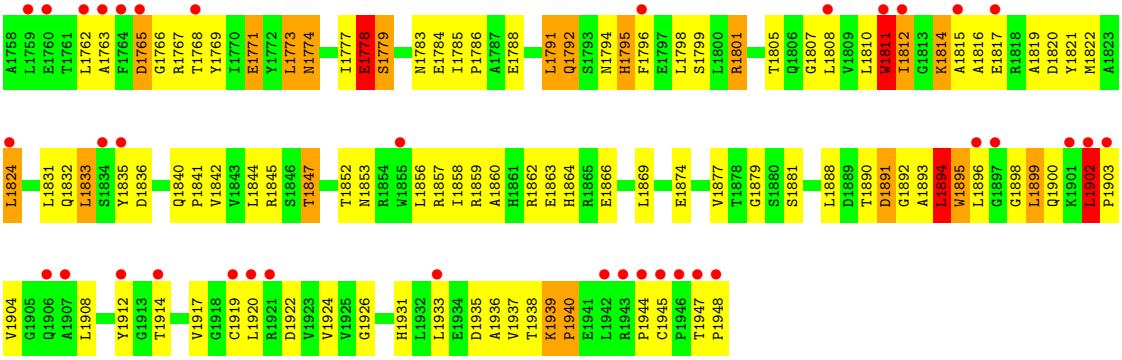
• Molecule 1: Agrin

Chain A:



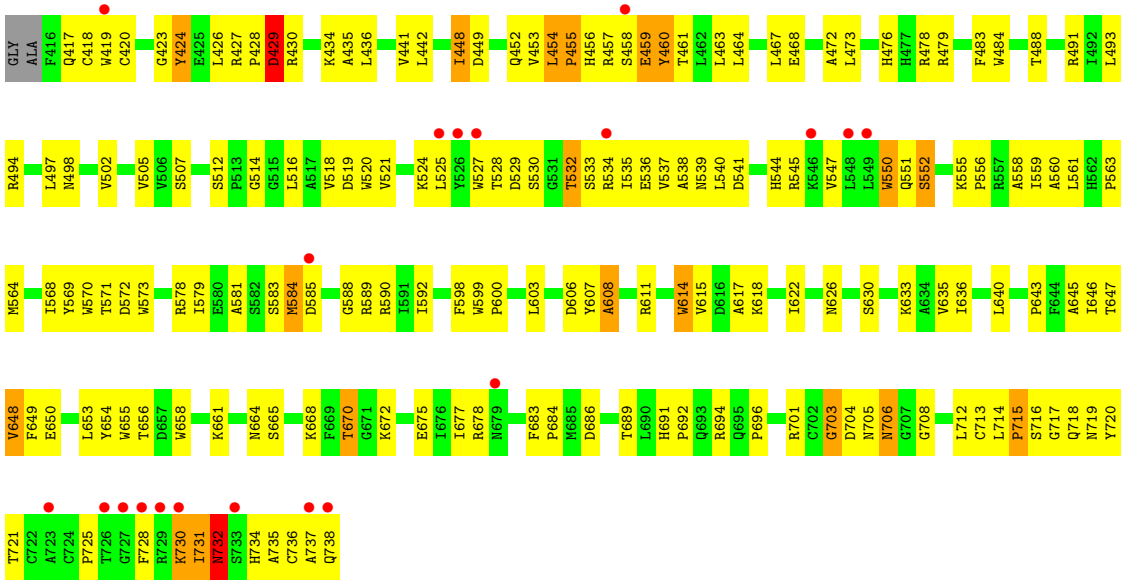
• Molecule 1: Agrin

Chain C:



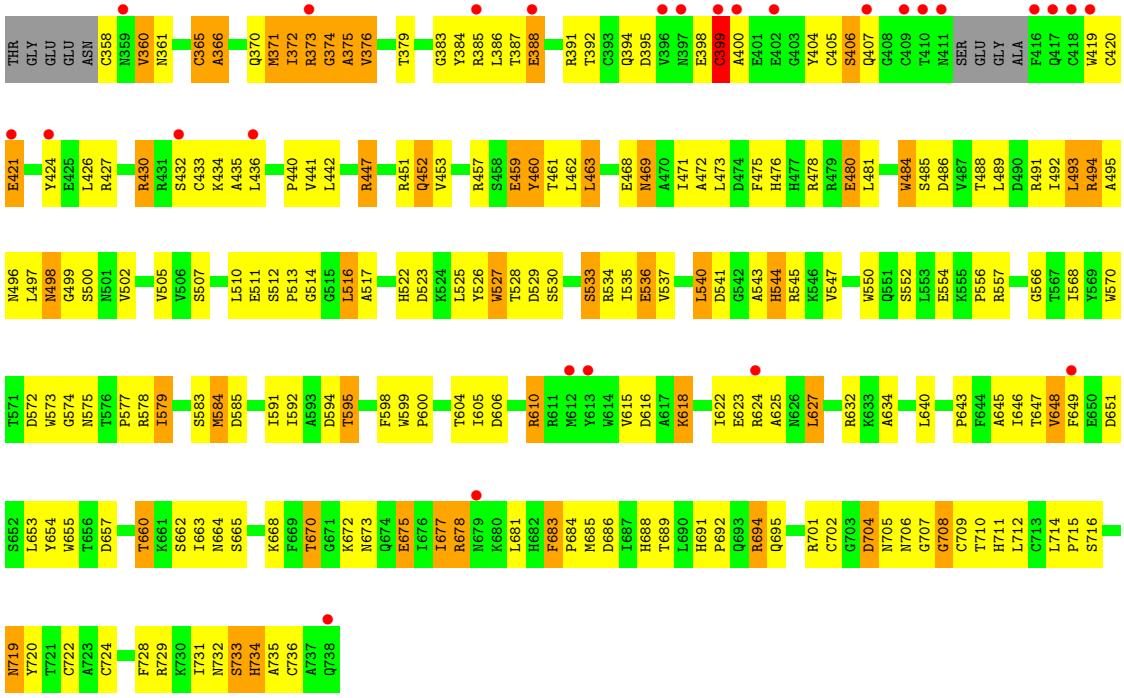
• Molecule 2: Low-density lipoprotein receptor-related protein 4

Chain B:



- Molecule 2: Low-density lipoprotein receptor-related protein 4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.72Å 110.23Å 158.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.30 57.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (60.00-3.30) 94.6 (57.48-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.297 0.242 , 0.311	Depositor DCC
R_{free} test set	1101 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	104.1	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: CA

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	0.51	0/1499	0.69	1/2041 (0.0%)
1	C	0.52	2/1499 (0.1%)	0.71	1/2041 (0.0%)
2	B	0.61	5/2711 (0.2%)	0.69	0/3684
2	D	0.60	4/3059 (0.1%)	0.71	1/4152 (0.0%)
All	All	0.57	11/8768 (0.1%)	0.70	3/11918 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	527	TRP	CD2-CE2	5.54	1.48	1.41
1	C	1895	TRP	CD2-CE2	5.42	1.47	1.41
1	C	1811	TRP	CD2-CE2	5.35	1.47	1.41
2	B	614	TRP	CD2-CE2	5.13	1.47	1.41
2	D	570	TRP	CD2-CE2	5.13	1.47	1.41
2	D	484	TRP	CD2-CE2	5.12	1.47	1.41
2	B	484	TRP	CD2-CE2	5.09	1.47	1.41
2	D	550	TRP	CD2-CE2	5.04	1.47	1.41
2	B	599	TRP	CD2-CE2	5.04	1.47	1.41
2	B	550	TRP	CD2-CE2	5.01	1.47	1.41
2	B	573	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	516	LEU	CA-CB-CG	-6.88	99.47	115.30
1	C	1894	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	1942	LEU	CA-CB-CG	5.09	127.02	115.30

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	1470	0	1474	65	0
1	C	1470	0	1474	90	0
2	B	2639	0	2536	145	1
2	D	2985	0	2844	179	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	8566	0	8328	471	1

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 28.

All (471) 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)
2:D:694:ARG:HG2	2:D:694:ARG:HH11	1.01	1.15
1:C:1773:LEU:H	1:C:1937:VAL:HG21	1.11	1.11
2:D:579:ILE:HG22	2:D:592:ILE:HB	1.30	1.07
2:D:453:VAL:HG12	2:D:460:TYR:HB2	1.11	1.06
2:D:705:ASN:OD1	2:D:708:GLY:HA3	1.59	1.03
1:C:1773:LEU:N	1:C:1937:VAL:HG21	1.75	1.01
2:B:622:ILE:HD13	2:B:636:ILE:HD12	1.45	0.95
2:B:476:HIS:ND1	2:B:479:ARG:HB2	1.81	0.94
2:B:691:HIS:ND1	2:B:692:PRO:HD2	1.84	0.93
2:B:468:GLU:HG3	2:B:488:THR:OG1	1.69	0.93
2:D:440:PRO:HG3	2:D:649:PHE:CE2	2.05	0.91
1:C:1769:TYR:HB3	1:C:1898:GLY:O	1.72	0.90
1:C:1763:ALA:HB1	1:C:1945:CYS:SG	2.11	0.89
2:D:610:ARG:HG3	2:D:610:ARG:HH11	1.39	0.88
2:B:532:THR:HG23	2:B:534:ARG:HE	1.37	0.88
1:C:1933:LEU:HA	1:C:1936:ALA:HB2	1.57	0.86
1:C:1768:THR:HG23	1:C:1940:PRO:HG2	1.58	0.86
2:B:524:LYS:HE2	2:B:712:LEU:HD22	1.58	0.86
2:D:528:THR:HG22	2:D:535:ILE:HG12	1.57	0.85
2:D:441:VAL:HG21	2:D:452:GLN:HG3	1.59	0.84
1:C:1794:ASN:O	1:C:1795:HIS:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:672:LYS:O	2:D:673:ASN:HB2	1.77	0.84
2:D:406:SER:HB3	2:D:432:SER:HA	1.62	0.81
2:D:694:ARG:HG2	2:D:694:ARG:NH1	1.79	0.81
2:D:705:ASN:OD1	2:D:708:GLY:CA	2.29	0.81
2:B:410:THR:HB	2:B:417:GLN:HE22	1.46	0.81
2:B:472:ALA:HB2	2:B:514:GLY:O	1.81	0.81
2:D:453:VAL:HG12	2:D:460:TYR:CB	2.04	0.80
2:B:407:GLN:HE21	2:B:608:ALA:HB1	1.46	0.80
2:B:716:SER:HB3	2:B:721:THR:HG23	1.65	0.79
2:B:537:VAL:HG22	2:B:538:ALA:H	1.49	0.77
1:C:1798:LEU:HD11	1:C:1920:LEU:HD23	1.66	0.77
2:B:658:TRP:O	2:B:661:LYS:HD3	1.85	0.77
2:D:711:HIS:CD2	2:D:736:CYS:HB2	2.20	0.77
2:D:663:ILE:HD12	2:D:681:LEU:HD11	1.66	0.77
1:C:1763:ALA:CB	1:C:1945:CYS:SG	2.73	0.76
2:D:610:ARG:HH11	2:D:610:ARG:CG	1.98	0.76
2:D:424:TYR:HB3	2:D:433:CYS:HB3	1.68	0.76
2:B:579:ILE:HD13	2:B:614:TRP:CD2	2.19	0.76
2:D:584:MET:HB2	2:D:715:PRO:O	1.86	0.75
2:D:716:SER:H	2:D:720:TYR:HA	1.51	0.75
1:A:1795:HIS:ND1	1:A:1861:HIS:HD2	1.84	0.74
2:B:603:LEU:HD12	2:B:614:TRP:HB3	1.69	0.74
2:B:656:THR:HB	2:B:684:PRO:HB2	1.69	0.74
1:A:1902:LEU:H	1:A:1903:PRO:HD3	1.52	0.74
1:C:1801:ARG:HD3	1:C:1853:ASN:HA	1.68	0.74
1:A:1771:GLU:HB2	1:A:1895:TRP:CE2	2.23	0.74
2:B:622:ILE:HD11	2:B:640:LEU:HD21	1.70	0.73
2:B:635:VAL:HG11	2:B:668:LYS:O	1.87	0.73
2:D:480:GLU:HA	2:D:497:LEU:HD12	1.71	0.73
1:C:1812:ILE:HG22	1:C:1822:MET:HG2	1.71	0.73
2:B:460:TYR:HA	2:B:678:ARG:HH12	1.53	0.72
1:A:1792:GLN:OE1	1:A:1864:HIS:NE2	2.22	0.72
1:C:1774:ASN:H	1:C:1893:ALA:HA	1.55	0.71
1:A:1842:VAL:HG13	1:A:1882:PRO:HD3	1.72	0.71
2:D:523:ASP:HB3	2:D:540:LEU:HD22	1.73	0.71
2:D:370:GLN:C	2:D:372:ILE:H	1.94	0.70
2:D:615:VAL:HG22	2:D:622:ILE:HG12	1.73	0.70
2:B:708:GLY:HA2	2:B:713:CYS:SG	2.31	0.70
2:B:528:THR:HG22	2:B:535:ILE:HG12	1.73	0.70
2:B:468:GLU:CG	2:B:488:THR:OG1	2.39	0.69
1:A:1826:ILE:HD11	1:A:1916:PHE:HE2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:GLU:O	2:D:399:CYS:HB2	1.92	0.69
2:D:694:ARG:HH11	2:D:694:ARG:CG	1.93	0.69
2:D:469:ASN:HB2	2:D:488:THR:HG23	1.73	0.69
2:B:691:HIS:HD1	2:B:692:PRO:HD2	1.56	0.69
2:B:532:THR:HG23	2:B:534:ARG:NE	2.08	0.69
2:D:469:ASN:CB	2:D:488:THR:HG23	2.23	0.69
2:D:657:ASP:HB3	2:D:660:THR:HG23	1.75	0.68
1:C:1812:ILE:HG13	1:C:1894:LEU:HB3	1.75	0.68
2:D:358:CYS:SG	2:D:371:MET:N	2.67	0.68
2:B:524:LYS:NZ	2:B:713:CYS:O	2.27	0.68
2:D:468:GLU:HG3	2:D:489:LEU:HD21	1.75	0.67
2:D:527:TRP:NE1	2:D:536:GLU:HG3	2.10	0.67
2:D:575:ASN:O	2:D:577:PRO:HD3	1.95	0.67
1:C:1812:ILE:CG2	1:C:1822:MET:HG2	2.25	0.67
2:D:554:GLU:HB2	2:D:574:GLY:HA3	1.75	0.67
2:D:598:PHE:HB3	2:D:618:LYS:HB3	1.75	0.66
1:C:1774:ASN:HB3	1:C:1892:GLY:C	2.14	0.66
2:B:731:ILE:O	2:B:732:ASN:HB2	1.95	0.66
2:B:537:VAL:HG22	2:B:538:ALA:N	2.10	0.66
1:C:1814:LYS:HE3	1:C:1891:ASP:HB3	1.77	0.66
1:C:1844:LEU:HD21	1:C:1879:GLY:HA3	1.78	0.66
1:A:1902:LEU:O	1:A:1904:VAL:HG13	1.95	0.66
1:A:1817:GLU:HG3	1:A:1905:GLY:HA2	1.78	0.65
1:A:1818:ARG:O	1:A:1818:ARG:HD3	1.97	0.65
2:D:358:CYS:N	2:D:361:ASN:HB2	2.10	0.65
2:D:566:GLY:C	2:D:584:MET:HG2	2.17	0.65
2:D:498:ASN:HB3	2:D:500:SER:OG	1.96	0.65
2:D:653:LEU:O	2:D:665:SER:HA	1.96	0.65
2:B:454:LEU:HD13	2:B:457:ARG:NH2	2.12	0.65
2:D:447:ARG:HH21	1:C:1786:PRO:HB2	1.63	0.64
1:A:1861:HIS:CE1	1:A:1863:GLU:HG2	2.32	0.64
1:C:1815:ALA:HB1	1:C:1904:VAL:HG11	1.79	0.64
1:A:1831:LEU:HG	1:A:1850:VAL:HG11	1.78	0.64
2:D:420:CYS:H	2:D:426:LEU:HD23	1.61	0.64
2:D:627:LEU:H	2:D:627:LEU:HD23	1.63	0.64
1:C:1771:GLU:HB3	1:C:1895:TRP:CE2	2.32	0.64
1:C:1824:LEU:HD11	1:C:1831:LEU:HD13	1.81	0.63
1:A:1792:GLN:OE1	1:C:1864:HIS:NE2	2.32	0.63
2:D:516:LEU:HD22	2:D:525:LEU:HD11	1.80	0.63
2:D:573:TRP:HB3	2:D:600:PRO:HD2	1.81	0.63
1:A:1801:ARG:HH22	1:A:1947:THR:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:ILE:HD11	2:B:653:LEU:HD22	1.81	0.63
1:C:1902:LEU:N	1:C:1903:PRO:HD2	2.14	0.63
2:B:448:ILE:O	2:B:467:LEU:HB2	1.99	0.63
2:D:701:ARG:NH1	2:D:719:ASN:O	2.32	0.63
2:D:366:ALA:HB2	2:D:391:ARG:O	1.98	0.62
2:D:681:LEU:HB2	2:D:684:PRO:HG3	1.80	0.62
2:B:407:GLN:NE2	2:B:608:ALA:HB1	2.12	0.62
2:D:579:ILE:HG22	2:D:592:ILE:CB	2.19	0.62
1:A:1861:HIS:HE1	1:A:1863:GLU:HG2	1.63	0.62
2:D:536:GLU:HB3	2:D:547:VAL:HA	1.82	0.62
2:D:704:ASP:OD1	2:D:704:ASP:N	2.32	0.62
1:A:1770:ILE:O	1:A:1895:TRP:HA	2.00	0.61
2:D:452:GLN:HE22	2:D:463:LEU:HD22	1.65	0.61
1:C:1857:ARG:HH22	1:C:1922:ASP:HB3	1.65	0.61
1:A:1811:TRP:CE3	1:A:1823:ALA:HB2	2.35	0.61
2:D:491:ARG:HD3	2:D:507:SER:HA	1.83	0.61
1:C:1771:GLU:HB3	1:C:1895:TRP:NE1	2.16	0.61
2:D:605:ILE:O	2:D:694:ARG:NH2	2.30	0.61
1:A:1902:LEU:N	1:A:1903:PRO:HD3	2.16	0.60
1:C:1771:GLU:HB3	1:C:1895:TRP:CD1	2.36	0.60
1:C:1824:LEU:HD11	1:C:1831:LEU:CD1	2.31	0.60
2:B:703:GLY:O	2:B:705:ASN:N	2.33	0.60
2:D:530:SER:HA	2:D:556:PRO:HD2	1.83	0.60
1:C:1816:ALA:HB3	1:C:1819:ALA:HB2	1.83	0.60
1:C:1807:GLY:HA2	1:C:1914:THR:OG1	2.01	0.60
2:B:454:LEU:HD13	2:B:457:ARG:HH21	1.66	0.60
2:B:560:ALA:HB3	2:B:569:TYR:HB2	1.83	0.60
2:D:405:CYS:O	2:D:407:GLN:N	2.34	0.60
2:D:627:LEU:N	2:D:627:LEU:CD2	2.64	0.60
2:B:713:CYS:HB2	2:B:720:TYR:HD1	1.67	0.60
2:D:405:CYS:O	2:D:406:SER:C	2.39	0.60
2:B:606:ASP:HB2	2:B:648:VAL:HG21	1.82	0.60
2:D:420:CYS:H	2:D:426:LEU:CD2	2.14	0.60
1:C:1779:SER:HB3	1:C:1784:GLU:O	2.02	0.59
2:B:455:PRO:O	2:B:677:ILE:HG12	2.03	0.59
2:D:374:GLY:O	2:D:375:ALA:HB2	2.01	0.59
1:C:1794:ASN:O	1:C:1795:HIS:CB	2.50	0.59
2:D:663:ILE:HD12	2:D:681:LEU:CD1	2.32	0.59
2:D:594:ASP:OD2	2:D:594:ASP:N	2.35	0.59
2:B:442:LEU:HB2	2:B:453:VAL:HG23	1.84	0.59
2:B:689:THR:HB	2:B:694:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:606:ASP:OD2	2:D:668:LYS:HE3	2.02	0.59
1:A:1794:ASN:OD1	1:A:1862:ARG:NH1	2.35	0.59
1:A:1857:ARG:HH12	1:A:1922:ASP:HB2	1.68	0.59
2:D:584:MET:HG3	2:D:715:PRO:HG2	1.83	0.59
2:D:716:SER:N	2:D:720:TYR:HA	2.16	0.59
1:C:1766:GLY:HA3	1:C:1917:VAL:HG13	1.83	0.59
1:C:1794:ASN:OD1	1:C:1862:ARG:NH1	2.36	0.59
1:A:1795:HIS:ND1	1:A:1861:HIS:CD2	2.71	0.58
2:B:452:GLN:HB2	2:B:461:THR:HB	1.86	0.58
2:B:564:MET:HE3	2:B:696:PRO:HG2	1.86	0.58
2:D:544:HIS:HB3	2:D:712:LEU:HD21	1.83	0.58
2:B:713:CYS:HB2	2:B:720:TYR:CD1	2.37	0.58
2:D:689:THR:HB	2:D:694:ARG:HD2	1.86	0.58
2:B:665:SER:HB3	2:B:677:ILE:CD1	2.34	0.58
2:D:610:ARG:C	2:D:627:LEU:HD21	2.24	0.58
2:D:655:TRP:CE2	2:D:664:ASN:HB2	2.39	0.57
1:C:1773:LEU:HB2	1:C:1937:VAL:CG2	2.34	0.57
2:D:440:PRO:HG3	2:D:649:PHE:HE2	1.64	0.57
2:D:598:PHE:CD2	2:D:618:LYS:HG2	2.40	0.57
2:B:521:VAL:HB	2:B:563:PRO:HB3	1.86	0.57
2:B:701:ARG:HG3	2:B:715:PRO:HB3	1.85	0.56
1:C:1792:GLN:HA	1:C:1862:ARG:NH2	2.19	0.56
2:B:460:TYR:HA	2:B:678:ARG:NH1	2.20	0.56
2:B:588:GLY:O	2:B:590:ARG:NH1	2.37	0.56
2:D:427:ARG:NE	2:D:434:LYS:HB2	2.20	0.56
2:D:453:VAL:CG1	2:D:460:TYR:HB2	2.07	0.56
2:B:491:ARG:HD3	2:B:507:SER:HA	1.86	0.56
2:B:427:ARG:O	2:B:429:ASP:N	2.38	0.56
2:B:463:LEU:HD23	2:B:464:LEU:HG	1.87	0.56
2:B:529:ASP:HB3	2:B:532:THR:HB	1.88	0.56
2:D:447:ARG:NH2	1:C:1786:PRO:HB2	2.20	0.56
2:B:423:GLY:C	2:B:424:TYR:HD2	2.09	0.56
1:C:1824:LEU:HD22	1:C:1833:LEU:HB2	1.86	0.56
1:C:1773:LEU:HB2	1:C:1937:VAL:HG21	1.87	0.56
1:C:1791:LEU:HD11	1:C:1890:THR:HB	1.86	0.56
1:A:1818:ARG:HH22	1:A:1907:ALA:HB1	1.71	0.55
1:C:1810:LEU:HD12	1:C:1896:LEU:HD13	1.87	0.55
2:B:569:TYR:HB3	2:B:603:LEU:HD21	1.88	0.55
2:D:365:CYS:O	2:D:365:CYS:SG	2.65	0.55
2:D:491:ARG:CD	2:D:507:SER:HA	2.37	0.55
1:C:1853:ASN:ND2	1:C:1948:PRO:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1908:LEU:HB3	1:C:1912:TYR:HB2	1.89	0.55
1:C:1832:GLN:HB3	1:C:1845:ARG:HG3	1.88	0.55
2:D:484:TRP:CE2	2:D:493:LEU:HD12	2.42	0.55
1:C:1795:HIS:CD2	1:C:1796:PHE:H	2.24	0.55
2:B:670:THR:HB	2:B:672:LYS:H	1.72	0.55
2:D:662:SER:HA	2:D:681:LEU:HD12	1.89	0.54
2:D:610:ARG:HG3	2:D:610:ARG:NH1	2.15	0.54
1:C:1811:TRP:CD1	1:C:1811:TRP:C	2.81	0.54
2:D:419:TRP:CZ3	2:D:421:GLU:HG2	2.43	0.54
1:A:1817:GLU:HG3	1:A:1905:GLY:CA	2.37	0.53
2:B:670:THR:HG21	2:B:672:LYS:HD2	1.89	0.53
2:B:734:HIS:CE1	2:B:735:ALA:HB2	2.43	0.53
2:D:384:TYR:O	2:D:386:LEU:N	2.41	0.53
2:D:469:ASN:HB2	2:D:488:THR:CG2	2.38	0.53
2:B:556:PRO:HA	2:B:571:THR:O	2.09	0.53
2:D:370:GLN:O	2:D:372:ILE:N	2.39	0.53
1:C:1902:LEU:H	1:C:1903:PRO:HD2	1.73	0.53
2:B:622:ILE:CD1	2:B:640:LEU:HD21	2.38	0.53
1:A:1801:ARG:NH1	1:A:1948:PRO:HD3	2.24	0.53
2:B:537:VAL:CG2	2:B:538:ALA:H	2.17	0.53
2:B:559:ILE:HD11	2:B:568:ILE:HD11	1.89	0.53
2:D:484:TRP:CZ2	2:D:493:LEU:HD13	2.44	0.53
2:B:649:PHE:CZ	2:B:691:HIS:CD2	2.96	0.53
1:C:1947:THR:OG1	1:C:1948:PRO:HD2	2.08	0.53
2:D:568:ILE:HD11	2:D:584:MET:HA	1.90	0.53
2:D:534:ARG:HD2	2:D:547:VAL:CG1	2.39	0.53
2:B:423:GLY:C	2:B:436:LEU:HG	2.29	0.52
2:B:598:PHE:HB3	2:B:618:LYS:HB3	1.91	0.52
2:D:578:ARG:HD2	2:D:591:ILE:HD12	1.90	0.52
1:A:1894:LEU:HD23	1:A:1895:TRP:N	2.25	0.52
2:D:517:ALA:HB3	2:D:526:TYR:HB2	1.90	0.52
1:A:1815:ALA:C	1:A:1904:VAL:HG11	2.29	0.52
2:B:731:ILE:HD12	2:B:737:ALA:HB3	1.90	0.52
2:D:371:MET:O	2:D:371:MET:HG2	2.10	0.52
2:D:677:ILE:HG22	2:D:678:ARG:N	2.25	0.52
1:A:1899:LEU:HB3	1:A:1902:LEU:HB2	1.92	0.52
2:B:418:CYS:HB2	2:B:430:ARG:O	2.09	0.52
1:C:1778:GLU:OE1	1:C:1778:GLU:N	2.43	0.52
1:A:1928:ARG:NH1	1:A:1935:ASP:OD2	2.42	0.52
2:B:472:ALA:HA	2:B:686:ASP:HB2	1.91	0.52
2:D:469:ASN:HD22	2:D:471:ILE:HD11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:LEU:H	2:D:627:LEU:CD2	2.23	0.52
1:C:1857:ARG:HG2	1:C:1859:ARG:HH12	1.75	0.52
2:D:724:CYS:HB3	2:D:728:PHE:HB2	1.92	0.51
2:D:372:ILE:HG22	2:D:373:ARG:H	1.75	0.51
2:D:526:TYR:CD2	2:D:537:VAL:HB	2.46	0.51
1:C:1821:TYR:CE2	1:C:1836:ASP:HB3	2.46	0.51
2:B:730:LYS:O	2:B:731:ILE:HB	2.10	0.51
2:B:728:PHE:HA	2:B:738:GLN:HA	1.92	0.51
2:D:732:ASN:O	2:D:734:HIS:N	2.44	0.51
1:C:1792:GLN:HG3	1:C:1864:HIS:NE2	2.26	0.51
1:C:1902:LEU:N	1:C:1903:PRO:CD	2.74	0.51
2:D:557:ARG:NH1	2:D:557:ARG:HG3	2.26	0.51
2:D:441:VAL:HG23	2:D:453:VAL:O	2.11	0.50
2:D:710:THR:OG1	2:D:735:ALA:HA	2.10	0.50
1:C:1832:GLN:HA	1:C:1845:ARG:HA	1.92	0.50
2:B:665:SER:HB3	2:B:677:ILE:HD11	1.93	0.50
2:D:622:ILE:HG13	2:D:640:LEU:HD11	1.92	0.50
2:B:648:VAL:HG23	2:B:694:ARG:NH1	2.27	0.50
2:D:522:HIS:CE1	2:D:715:PRO:HG3	2.47	0.50
1:A:1902:LEU:N	1:A:1903:PRO:CD	2.73	0.50
2:D:654:TYR:CD2	2:D:665:SER:HB3	2.47	0.50
1:A:1927:HIS:CE1	1:C:1795:HIS:HB3	2.47	0.50
1:A:1931:HIS:HB3	1:A:1934:GLU:HG2	1.94	0.50
2:B:564:MET:SD	2:B:564:MET:N	2.83	0.50
2:B:579:ILE:HD13	2:B:614:TRP:CE3	2.46	0.50
2:D:468:GLU:HB2	2:D:486:ASP:OD1	2.12	0.50
1:C:1812:ILE:CD1	1:C:1894:LEU:HG	2.41	0.50
1:A:1771:GLU:HB2	1:A:1895:TRP:CZ2	2.46	0.49
1:A:1846:SER:OG	1:A:1848:VAL:HB	2.11	0.49
2:D:386:LEU:HD22	2:D:388:GLU:OE2	2.13	0.49
2:B:579:ILE:HG22	2:B:592:ILE:HB	1.94	0.49
1:C:1812:ILE:HD12	1:C:1894:LEU:HG	1.93	0.49
2:D:420:CYS:HB3	2:D:424:TYR:HB2	1.95	0.49
2:D:645:ALA:O	2:D:655:TRP:HA	2.13	0.49
2:B:559:ILE:HA	2:B:569:TYR:O	2.12	0.49
2:D:572:ASP:O	2:D:577:PRO:HA	2.13	0.49
2:D:624:ARG:O	2:D:632:ARG:HA	2.13	0.49
1:C:1902:LEU:H	1:C:1903:PRO:CD	2.25	0.49
1:A:1846:SER:CB	1:A:1871:VAL:HG21	2.42	0.49
1:C:1773:LEU:HD22	1:C:1893:ALA:HB2	1.94	0.49
2:B:533:SER:C	2:B:534:ARG:HG3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:LEU:CD2	2:B:568:ILE:HG13	2.43	0.48
1:C:1808:LEU:HD13	1:C:1912:TYR:HD2	1.78	0.48
2:B:536:GLU:HG2	2:B:547:VAL:HA	1.95	0.48
2:D:710:THR:OG1	2:D:734:HIS:O	2.26	0.48
2:B:538:ALA:HB2	2:B:545:ARG:HG2	1.93	0.48
2:B:649:PHE:CZ	2:B:691:HIS:HD2	2.31	0.48
2:B:649:PHE:HZ	2:B:691:HIS:CD2	2.30	0.48
1:A:1793:SER:HA	1:A:1862:ARG:O	2.13	0.48
2:B:569:TYR:CD2	2:B:581:ALA:HB2	2.48	0.48
2:D:516:LEU:HA	2:D:516:LEU:HD23	1.37	0.48
1:C:1774:ASN:HD22	1:C:1892:GLY:HA2	1.79	0.48
2:B:423:GLY:C	2:B:424:TYR:CD2	2.87	0.48
2:B:527:TRP:CZ2	2:B:536:GLU:HB2	2.49	0.48
2:D:615:VAL:HG11	2:D:643:PRO:HB2	1.96	0.48
1:A:1846:SER:HB2	1:A:1871:VAL:CG2	2.44	0.48
1:C:1796:PHE:HB3	1:C:1924:VAL:O	2.13	0.48
2:B:468:GLU:HG3	2:B:488:THR:HG1	1.77	0.48
2:B:617:ALA:HA	2:B:643:PRO:HD2	1.94	0.48
1:A:1865:ARG:HG2	1:A:1881:SER:OG	2.14	0.48
2:B:647:THR:HG22	2:B:654:TYR:HB2	1.96	0.47
1:A:1894:LEU:HD23	1:A:1894:LEU:C	2.35	0.47
2:B:456:HIS:CE1	2:B:675:GLU:OE2	2.67	0.47
2:D:469:ASN:ND2	2:D:471:ILE:HD11	2.29	0.47
2:B:670:THR:HG21	2:B:672:LYS:CD	2.43	0.47
1:A:1840:GLN:HB2	1:A:1882:PRO:HG2	1.97	0.47
2:D:496:ASN:O	2:D:499:GLY:N	2.47	0.47
2:D:715:PRO:HA	2:D:720:TYR:HA	1.95	0.47
1:A:1810:LEU:HD23	1:A:1811:TRP:N	2.29	0.47
1:C:1763:ALA:HB3	1:C:1945:CYS:N	2.30	0.47
2:B:476:HIS:ND1	2:B:478:ARG:O	2.48	0.47
2:D:647:THR:CG2	2:D:654:TYR:HB2	2.45	0.47
1:C:1815:ALA:HB1	1:C:1904:VAL:CG1	2.45	0.47
2:B:476:HIS:CD2	2:B:520:TRP:HA	2.50	0.47
1:C:1765:ASP:HB2	1:C:1768:THR:OG1	2.15	0.47
1:C:1795:HIS:CD2	1:C:1796:PHE:N	2.83	0.47
2:D:374:GLY:O	2:D:375:ALA:CB	2.63	0.46
2:D:492:ILE:HG13	2:D:510:LEU:CD1	2.45	0.46
1:A:1919:CYS:O	1:A:1920:LEU:HD12	2.15	0.46
2:B:544:HIS:ND1	2:B:712:LEU:HG	2.30	0.46
2:B:525:LEU:HD23	2:B:525:LEU:C	2.36	0.46
2:D:557:ARG:HG3	2:D:557:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:651:ASP:HA	2:D:668:LYS:HD3	1.97	0.46
2:D:370:GLN:C	2:D:372:ILE:N	2.61	0.46
2:D:471:ILE:HD12	2:D:685:MET:HG3	1.98	0.46
2:D:475:PHE:CE1	2:D:695:GLN:NE2	2.84	0.46
1:A:1830:HIS:HB2	1:A:1845:ARG:NH2	2.30	0.46
2:D:533:SER:OG	2:D:554:GLU:O	2.34	0.46
2:B:585:ASP:OD2	2:B:716:SER:HB2	2.15	0.46
2:B:731:ILE:O	2:B:732:ASN:CB	2.63	0.46
2:D:471:ILE:HG13	1:C:1785:ILE:HG21	1.97	0.46
1:A:1806:GLN:NE2	1:A:1828:ASP:H	2.14	0.46
2:B:457:ARG:HB3	2:B:459:GLU:H	1.81	0.46
1:C:1763:ALA:H	1:C:1944:PRO:HA	1.80	0.46
1:A:1818:ARG:HA	1:A:1818:ARG:NH1	2.30	0.45
2:D:472:ALA:HB2	2:D:514:GLY:O	2.16	0.45
2:D:485:SER:HA	2:D:492:ILE:HA	1.98	0.45
2:D:599:TRP:O	2:D:616:ASP:HA	2.17	0.45
2:D:702:CYS:O	2:D:707:GLY:HA3	2.16	0.45
1:A:1827:VAL:HG22	1:A:1911:ALA:HB3	1.99	0.45
2:B:530:SER:HA	2:B:556:PRO:HD2	1.99	0.45
2:B:615:VAL:HG22	2:B:622:ILE:HG13	1.98	0.45
2:B:600:PRO:HA	2:B:615:VAL:O	2.16	0.45
2:D:452:GLN:HE22	2:D:463:LEU:CD2	2.30	0.45
2:D:471:ILE:CD1	2:D:685:MET:HG3	2.47	0.45
2:D:604:THR:HG23	2:D:648:VAL:HG22	1.98	0.45
2:B:434:LYS:HG2	2:B:435:ALA:N	2.32	0.45
2:D:657:ASP:HB3	2:D:660:THR:CG2	2.46	0.45
2:D:554:GLU:CB	2:D:574:GLY:HA3	2.45	0.45
2:D:691:HIS:CG	2:D:692:PRO:HD2	2.52	0.45
2:D:583:SER:O	2:D:585:ASP:N	2.49	0.44
2:B:555:LYS:N	2:B:572:ASP:OD2	2.50	0.44
2:D:394:GLN:HB3	2:D:395:ASP:H	1.58	0.44
2:D:665:SER:OG	2:D:675:GLU:HB3	2.17	0.44
2:B:718:GLN:N	2:B:718:GLN:CD	2.71	0.44
1:A:1883:LEU:HD23	2:D:534:ARG:NH1	2.32	0.44
2:B:585:ASP:HA	2:B:714:LEU:HD13	1.99	0.44
2:D:494:ARG:HH21	2:D:541:ASP:HA	1.82	0.44
1:C:1857:ARG:HG2	1:C:1859:ARG:NH1	2.32	0.44
2:B:483:PHE:CD1	2:B:518:VAL:HG21	2.53	0.44
2:B:532:THR:O	2:B:534:ARG:HG3	2.18	0.44
2:D:476:HIS:HB3	2:D:481:LEU:HB2	1.99	0.44
2:B:708:GLY:CA	2:B:713:CYS:SG	3.03	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:670:THR:C	2:D:672:LYS:H	2.21	0.44
2:B:552:SER:HB2	2:B:589:ARG:NH2	2.33	0.44
2:D:681:LEU:H	2:D:681:LEU:HG	1.66	0.44
2:B:404:TYR:N	2:B:404:TYR:CD2	2.86	0.44
2:B:731:ILE:O	2:B:731:ILE:HG22	2.18	0.44
2:D:722:CYS:HB2	2:D:733:SER:O	2.17	0.43
1:A:1801:ARG:NH2	1:A:1947:THR:HA	2.32	0.43
2:D:624:ARG:HG2	2:D:625:ALA:N	2.33	0.43
1:C:1853:ASN:HD22	1:C:1948:PRO:HB3	1.82	0.43
2:B:622:ILE:HD12	2:B:640:LEU:HD11	2.00	0.43
2:B:706:ASN:O	2:B:708:GLY:N	2.49	0.43
2:D:387:THR:O	2:D:388:GLU:C	2.57	0.43
1:C:1779:SER:O	1:C:1783:ASN:N	2.31	0.43
1:C:1792:GLN:HG3	1:C:1864:HIS:CE1	2.54	0.43
1:C:1799:SER:HA	1:C:1857:ARG:HA	2.00	0.43
2:B:519:ASP:HB2	2:B:561:LEU:HD13	2.01	0.43
1:C:1773:LEU:H	1:C:1937:VAL:CG2	2.02	0.43
1:A:1773:LEU:HG	1:A:1937:VAL:HG21	2.00	0.43
2:B:552:SER:HB3	2:B:578:ARG:HH12	1.83	0.43
2:D:485:SER:HB2	2:D:513:PRO:HB2	1.99	0.43
2:D:728:PHE:N	2:D:728:PHE:CD2	2.86	0.43
1:A:1802:THR:OG1	1:A:1917:VAL:O	2.36	0.43
1:A:1818:ARG:HH22	1:A:1907:ALA:CB	2.31	0.43
2:D:494:ARG:NH2	2:D:541:ASP:HA	2.34	0.43
2:D:566:GLY:CA	2:D:584:MET:HG2	2.49	0.43
1:A:1931:HIS:O	1:A:1935:ASP:HB2	2.19	0.43
2:B:424:TYR:CD2	2:B:424:TYR:N	2.87	0.43
2:B:453:VAL:HG11	2:B:678:ARG:HD3	1.99	0.43
1:A:1859:ARG:O	1:A:1869:LEU:HA	2.19	0.43
2:B:560:ALA:O	2:B:569:TYR:N	2.48	0.43
2:B:626:ASN:HB2	2:B:630:SER:O	2.19	0.43
2:D:494:ARG:HB3	2:D:505:VAL:CG2	2.48	0.43
2:D:625:ALA:HB2	2:D:632:ARG:HB2	2.01	0.43
1:C:1836:ASP:HB2	1:C:1841:PRO:HB3	2.01	0.43
2:B:615:VAL:HG13	2:B:643:PRO:HG2	2.00	0.43
2:D:715:PRO:HA	2:D:720:TYR:CB	2.49	0.43
1:A:1839:SER:H	1:A:1885:ALA:CB	2.32	0.42
2:B:454:LEU:HA	2:B:455:PRO:HD2	1.70	0.42
2:B:583:SER:O	2:B:585:ASP:N	2.52	0.42
2:B:607:TYR:CD2	2:B:696:PRO:HG3	2.54	0.42
2:D:407:GLN:HG3	2:D:420:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:424:TYR:CD1	2:D:435:ALA:HA	2.54	0.42
1:C:1821:TYR:HE2	1:C:1836:ASP:HB3	1.83	0.42
1:A:1781:LEU:HD23	1:A:1781:LEU:HA	1.86	0.42
2:B:521:VAL:HG21	2:B:563:PRO:HB2	2.01	0.42
2:B:534:ARG:HG2	2:B:550:TRP:HA	2.01	0.42
2:B:537:VAL:CG2	2:B:538:ALA:N	2.77	0.42
2:B:653:LEU:O	2:B:665:SER:HA	2.20	0.42
2:D:492:ILE:HG23	2:D:516:LEU:HD11	2.01	0.42
1:A:1846:SER:C	1:A:1848:VAL:H	2.22	0.42
2:B:654:TYR:CD2	2:B:677:ILE:CD1	3.02	0.42
2:B:655:TRP:CE2	2:B:664:ASN:HB2	2.54	0.42
2:B:429:ASP:OD1	2:B:430:ARG:N	2.53	0.42
2:D:441:VAL:CG2	2:D:452:GLN:HG3	2.42	0.42
2:D:492:ILE:HG13	2:D:510:LEU:HD11	2.02	0.42
2:B:561:LEU:HB3	2:B:584:MET:HE2	2.02	0.42
2:D:646:ILE:HD12	2:D:655:TRP:HB3	2.00	0.42
2:D:388:GLU:OE1	2:D:388:GLU:N	2.53	0.42
2:D:655:TRP:NE1	2:D:664:ASN:HB2	2.35	0.42
1:C:1847:THR:HG23	1:C:1874:GLU:HG3	2.02	0.42
1:C:1895:TRP:CZ3	1:C:1899:LEU:HG	2.55	0.42
1:A:1818:ARG:O	1:A:1819:ALA:C	2.58	0.41
2:D:705:ASN:HA	2:D:708:GLY:H	1.85	0.41
1:A:1865:ARG:HD2	1:A:1883:LEU:HA	2.02	0.41
2:B:476:HIS:CE1	2:B:479:ARG:HB2	2.50	0.41
1:A:1762:LEU:HD12	1:A:1932:LEU:HD22	2.03	0.41
1:A:1801:ARG:CZ	1:A:1948:PRO:HD3	2.50	0.41
2:B:420:CYS:SG	2:B:426:LEU:N	2.93	0.41
2:D:462:LEU:HD23	2:D:463:LEU:N	2.34	0.41
2:D:512:SER:O	2:D:529:ASP:HA	2.20	0.41
2:B:539:ASN:HB3	2:B:541:ASP:OD2	2.21	0.41
2:D:728:PHE:N	2:D:728:PHE:HD2	2.18	0.41
1:C:1766:GLY:C	1:C:1768:THR:H	2.24	0.41
2:D:595:THR:O	2:D:632:ARG:NH2	2.42	0.41
2:D:647:THR:HG22	2:D:654:TYR:HB2	2.02	0.41
1:C:1796:PHE:CZ	1:C:1860:ALA:HB3	2.55	0.41
1:C:1939:LYS:HA	1:C:1940:PRO:HD3	1.84	0.41
1:A:1769:TYR:CD2	1:A:1900:GLN:HB2	2.55	0.41
1:A:1896:LEU:HD12	1:A:1896:LEU:HA	1.88	0.41
2:B:527:TRP:CE2	2:B:536:GLU:HB2	2.56	0.41
2:B:532:THR:CG2	2:B:534:ARG:HB2	2.50	0.41
2:B:649:PHE:CE2	2:B:650:GLU:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:714:LEU:HA	2:D:715:PRO:HD2	1.95	0.41
2:D:719:ASN:HB3	2:D:720:TYR:H	1.60	0.41
1:C:1899:LEU:CD2	1:C:1900:GLN:H	2.33	0.41
1:C:1931:HIS:HB2	1:C:1935:ASP:OD2	2.21	0.41
2:D:457:ARG:C	2:D:459:GLU:H	2.24	0.41
2:D:623:GLU:HA	2:D:634:ALA:HA	2.01	0.41
1:A:1796:PHE:CD2	1:A:1796:PHE:C	2.94	0.41
2:B:550:TRP:CZ3	2:B:551:GLN:HG2	2.56	0.41
2:D:534:ARG:HD2	2:D:547:VAL:HG13	2.02	0.41
2:B:525:LEU:CD2	2:B:527:TRP:HE3	2.33	0.41
2:B:716:SER:CB	2:B:721:THR:HG23	2.43	0.41
2:D:388:GLU:H	2:D:388:GLU:CD	2.23	0.41
2:D:511:GLU:N	2:D:529:ASP:OD2	2.44	0.41
1:C:1812:ILE:HG13	1:C:1894:LEU:CB	2.49	0.41
1:C:1822:MET:CB	1:C:1835:TYR:HB3	2.51	0.41
1:A:1868:SER:HB2	1:A:1878:THR:HG22	2.02	0.41
2:B:478:ARG:O	2:B:479:ARG:HB2	2.21	0.41
1:C:1822:MET:HB2	1:C:1835:TYR:HB3	2.02	0.41
1:A:1857:ARG:NH1	1:A:1922:ASP:HB2	2.34	0.40
2:D:484:TRP:CZ2	2:D:493:LEU:CD1	3.04	0.40
2:D:495:ALA:HB2	2:D:502:VAL:HG12	2.02	0.40
2:D:645:ALA:CB	2:D:686:ASP:HA	2.51	0.40
1:A:1927:HIS:HE1	1:C:1926:GLY:O	2.04	0.40
2:B:483:PHE:CD2	2:B:494:ARG:HB3	2.56	0.40
1:C:1810:LEU:HD21	1:C:1812:ILE:HD12	2.02	0.40
2:B:555:LYS:O	2:B:572:ASP:HA	2.21	0.40
2:B:661:LYS:HA	2:B:661:LYS:HD2	1.89	0.40
2:D:360:VAL:HG13	2:D:361:ASN:ND2	2.36	0.40
2:D:372:ILE:O	2:D:374:GLY:N	2.54	0.40
2:B:525:LEU:CD2	2:B:527:TRP:CE3	3.04	0.40
2:B:558:ALA:O	2:B:570:TRP:HA	2.21	0.40
2:D:391:ARG:HD2	2:D:391:ARG:N	2.37	0.40
1:C:1791:LEU:CD1	1:C:1888:LEU:HD23	2.52	0.40
1:C:1844:LEU:HD22	1:C:1877:VAL:HG12	2.02	0.40
1:A:1792:GLN:HG3	1:C:1863:GLU:OE2	2.22	0.40
2:B:424:TYR:HD2	2:B:424:TYR:N	2.19	0.40
2:B:476:HIS:ND1	2:B:479:ARG:CB	2.68	0.40
2:B:645:ALA:O	2:B:655:TRP:HB2	2.21	0.40
2:D:398:GLU:O	2:D:399:CYS:CB	2.66	0.40
2:D:578:ARG:HD2	2:D:591:ILE:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:TRP:CH2	2:D:543:ALA:CB[4_455]	2.15	0.05

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	189/191 (99%)	165 (87%)	18 (10%)	6 (3%)	4 22
1	C	189/191 (99%)	150 (79%)	31 (16%)	8 (4%)	3 17
2	B	326/386 (84%)	262 (80%)	46 (14%)	18 (6%)	2 11
2	D	373/386 (97%)	295 (79%)	55 (15%)	23 (6%)	1 10
All	All	1077/1154 (93%)	872 (81%)	150 (14%)	55 (5%)	2 13

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1774	ASN
1	A	1940	PRO
2	B	704	ASP
2	B	706	ASN
2	B	731	ILE
2	D	360	VAL
2	D	375	ALA
2	D	385	ARG
2	D	388	GLU
2	D	399	CYS
2	D	406	SER
2	D	584	MET
1	C	1795	HIS
2	B	429	ASP
2	B	703	GLY
2	B	717	GLY

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Mol	Chain	Res	Type
2	B	732	ASN
2	D	430	ARG
2	D	708	GLY
1	C	1778	GLU
1	C	1852	THR
1	A	1916	PHE
2	B	428	PRO
2	B	552	SER
2	B	584	MET
2	B	719	ASN
2	B	730	LYS
2	D	373	ARG
2	D	709	CYS
1	C	1774	ASN
1	C	1820	ASP
1	C	1940	PRO
2	B	455	PRO
2	B	459	GLU
2	B	498	ASN
2	D	376	VAL
2	D	447	ARG
2	D	683	PHE
2	D	733	SER
1	A	1902	LEU
1	A	1917	VAL
2	B	608	ALA
2	B	715	PRO
2	B	725	PRO
2	D	366	ALA
2	D	371	MET
2	D	372	ILE
2	D	374	GLY
2	D	400	ALA
2	D	478	ARG
1	C	1840	GLN
1	C	1902	LEU
1	A	1907	ALA
2	D	383	GLY
2	D	677	ILE

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	156/156 (100%)	145 (93%)	11 (7%)	14	42
1	C	156/156 (100%)	123 (79%)	33 (21%)	1	4
2	B	283/327 (86%)	258 (91%)	25 (9%)	10	33
2	D	321/327 (98%)	274 (85%)	47 (15%)	3	14
All	All	916/966 (95%)	800 (87%)	116 (13%)	4	19

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1759	LEU
1	A	1776	VAL
1	A	1791	LEU
1	A	1792	GLN
1	A	1796	PHE
1	A	1818	ARG
1	A	1842	VAL
1	A	1896	LEU
1	A	1901	LYS
1	A	1919	CYS
1	A	1928	ARG
2	B	409	CYS
2	B	424	TYR
2	B	429	ASP
2	B	441	VAL
2	B	448	ILE
2	B	449	ASP
2	B	454	LEU
2	B	458	SER
2	B	460	TYR
2	B	473	LEU
2	B	493	LEU
2	B	497	LEU
2	B	502	VAL

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Mol	Chain	Res	Type
2	B	505	VAL
2	B	512	SER
2	B	516	LEU
2	B	532	THR
2	B	540	LEU
2	B	611	ARG
2	B	633	LYS
2	B	648	VAL
2	B	670	THR
2	B	683	PHE
2	B	732	ASN
2	B	736	CYS
2	D	365	CYS
2	D	376	VAL
2	D	379	THR
2	D	392	THR
2	D	399	CYS
2	D	404	TYR
2	D	421	GLU
2	D	430	ARG
2	D	436	LEU
2	D	442	LEU
2	D	451	ARG
2	D	452	GLN
2	D	459	GLU
2	D	460	TYR
2	D	461	THR
2	D	463	LEU
2	D	469	ASN
2	D	473	LEU
2	D	480	GLU
2	D	493	LEU
2	D	494	ARG
2	D	498	ASN
2	D	533	SER
2	D	536	GLU
2	D	540	LEU
2	D	544	HIS
2	D	545	ARG
2	D	552	SER
2	D	579	ILE
2	D	595	THR

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Mol	Chain	Res	Type
2	D	610	ARG
2	D	618	LYS
2	D	627	LEU
2	D	648	VAL
2	D	660	THR
2	D	670	THR
2	D	675	GLU
2	D	678	ARG
2	D	683	PHE
2	D	688	HIS
2	D	694	ARG
2	D	704	ASP
2	D	706	ASN
2	D	719	ASN
2	D	729	ARG
2	D	731	ILE
2	D	734	HIS
1	C	1762	LEU
1	C	1765	ASP
1	C	1767	ARG
1	C	1771	GLU
1	C	1773	LEU
1	C	1777	ILE
1	C	1778	GLU
1	C	1779	SER
1	C	1788	GLU
1	C	1791	LEU
1	C	1792	GLN
1	C	1801	ARG
1	C	1805	THR
1	C	1811	TRP
1	C	1812	ILE
1	C	1814	LYS
1	C	1817	GLU
1	C	1824	LEU
1	C	1833	LEU
1	C	1842	VAL
1	C	1847	THR
1	C	1856	LEU
1	C	1858	ILE
1	C	1866	GLU
1	C	1869	LEU

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Mol	Chain	Res	Type
1	C	1881	SER
1	C	1891	ASP
1	C	1894	LEU
1	C	1899	LEU
1	C	1902	LEU
1	C	1919	CYS
1	C	1938	THR
1	C	1939	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1861	HIS
1	A	1927	HIS
2	B	407	GLN
2	B	642	HIS
2	B	691	HIS
2	B	711	HIS
2	D	361	ASN
2	D	452	GLN
2	D	469	ASN
2	D	562	HIS
2	D	664	ASN
2	D	674	GLN
2	D	711	HIS
1	C	1774	ASN
1	C	1861	HIS
1	C	1927	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 (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	191/191 (100%)	0.55	19 (9%)	7	7	48, 78, 138, 167	0
1	C	191/191 (100%)	1.09	37 (19%)	1	1	35, 121, 178, 240	0
2	B	330/386 (85%)	0.44	20 (6%)	21	20	34, 66, 125, 169	0
2	D	377/386 (97%)	0.34	27 (7%)	15	15	30, 65, 139, 240	0
All	All	1089/1154 (94%)	0.54	103 (9%)	8	8	30, 75, 152, 240	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1906	GLN	8.6
2	B	738	GLN	7.6
2	B	726	THR	6.9
1	C	1947	THR	6.9
1	A	1945	CYS	6.7
1	A	1948	PRO	6.3
1	C	1948	PRO	6.2
1	C	1768	THR	5.8
1	C	1920	LEU	5.3
2	D	738	GLN	5.2
2	D	418	CYS	5.1
2	D	419	TRP	5.1
1	C	1946	PRO	4.6
1	A	1944	PRO	4.6
1	C	1907	ALA	4.4
2	D	416	PHE	4.3
2	D	411	ASN	4.3
2	B	729	ARG	4.2
2	D	397	ASN	4.2
1	C	1914	THR	4.1
1	C	1824	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	728	PHE	4.1
1	C	1933	LEU	4.1
1	C	1902	LEU	3.9
2	D	409	CYS	3.9
1	C	1759	LEU	3.9
1	C	1835	TYR	3.9
2	B	727	GLY	3.8
1	C	1764	PHE	3.7
2	D	613	TYR	3.6
1	C	1944	PRO	3.6
1	A	1768	THR	3.5
2	B	419	TRP	3.5
2	B	526	TYR	3.4
2	D	432	SER	3.4
1	A	1940	PRO	3.4
1	C	1763	ALA	3.3
1	C	1945	CYS	3.3
1	C	1815	ALA	3.2
2	D	410	THR	3.2
1	A	1900	GLN	3.2
1	C	1903	PRO	3.1
1	C	1912	TYR	3.1
1	C	1762	LEU	3.1
1	A	1833	LEU	3.1
2	B	723	ALA	3.1
2	D	649	PHE	3.0
1	A	1831	LEU	3.0
2	D	399	CYS	2.9
2	D	424	TYR	2.9
1	C	1765	ASP	2.9
1	A	1850	VAL	2.9
1	A	1946	PRO	2.8
1	A	1769	TYR	2.8
2	D	436	LEU	2.8
1	C	1834	SER	2.7
1	A	1824	LEU	2.7
2	B	458	SER	2.7
2	B	548	LEU	2.7
2	B	737	ALA	2.6
2	D	417	GLN	2.6
1	C	1855	TRP	2.5
1	C	1919	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	585	ASP	2.5
2	B	679	ASN	2.5
1	A	1901	LYS	2.5
2	B	534	ARG	2.5
2	D	612	MET	2.5
2	D	400	ALA	2.5
2	D	679	ASN	2.4
1	C	1943	ARG	2.4
2	D	385	ARG	2.4
1	C	1808	LEU	2.3
1	A	1906	GLN	2.3
2	D	421	GLU	2.3
2	D	407	GLN	2.3
2	B	525	LEU	2.3
1	C	1897	GLY	2.3
2	B	730	LYS	2.3
1	C	1812	ILE	2.3
2	B	527	TRP	2.3
2	D	359	ASN	2.3
1	A	1942	LEU	2.2
1	C	1811	TRP	2.2
2	D	396	VAL	2.2
2	D	402	GLU	2.2
2	D	624	ARG	2.2
1	C	1942	LEU	2.2
1	C	1796	PHE	2.2
2	D	388	GLU	2.2
1	C	1817	GLU	2.1
1	C	1896	LEU	2.1
1	C	1921	ARG	2.1
2	B	733	SER	2.1
1	C	1901	LYS	2.1
1	A	1832	GLN	2.1
2	B	549	LEU	2.1
1	A	1802	THR	2.1
1	A	1941	GLU	2.1
1	C	1760	GLU	2.0
2	B	546	LYS	2.0
1	A	1943	ARG	2.0
2	D	373	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	CA	C	2001	1/1	0.51	0.27	143,143,143,143	0
3	CA	A	2001	1/1	0.96	0.38	98,98,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.