Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:50 AM GMT

PDB ID	:	2V0V
Title	:	CRYSTAL STRUCTURE OF REV-ERB BETA
Authors	:	Woo, E.-J.; Jeong, D.G.; Lim, M.-Y.; Jun Kim, S.; Eon Ryu, S.
Deposited on	:	2007-05-19
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

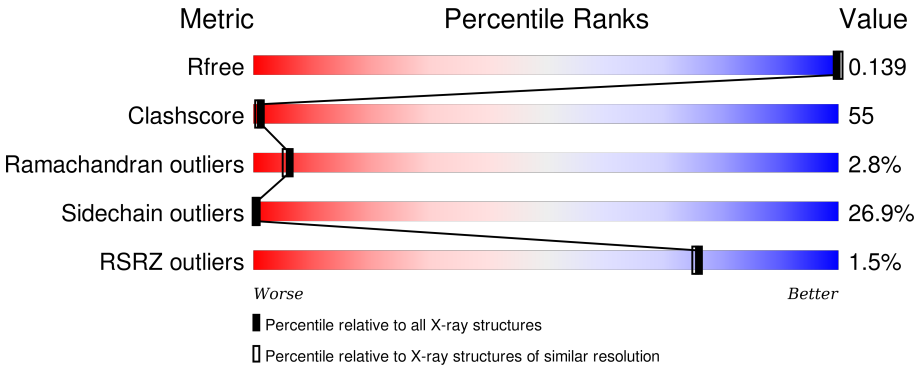
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 >=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 <=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	194	26% 51% 14% • 7%
1	B	194	26% 49% 17% • 7%
1	C	194	26% 47% 20% 8%
1	D	194	21% 50% 21% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5810 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 ORPHAN NUCLEAR RECEPTOR NR1D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1436	915	241	273	7			
1	B	181	Total	C	N	O	S	0	0	0
			1436	915	241	273	7			
1	C	179	Total	C	N	O	S	0	0	0
			1421	906	238	270	7			
1	D	179	Total	C	N	O	S	0	0	0
			1421	906	238	270	7			

- Molecule 2 is water.

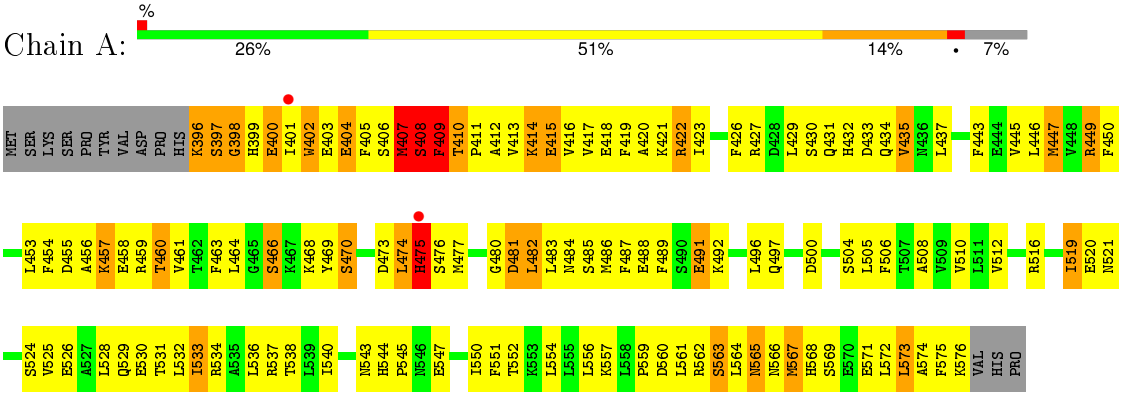
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	26	Total	O	0	0
			26	26		
2	C	22	Total	O	0	0
			22	22		
2	D	25	Total	O	0	0
			25	25		

3 Residue-property plots (i)

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.

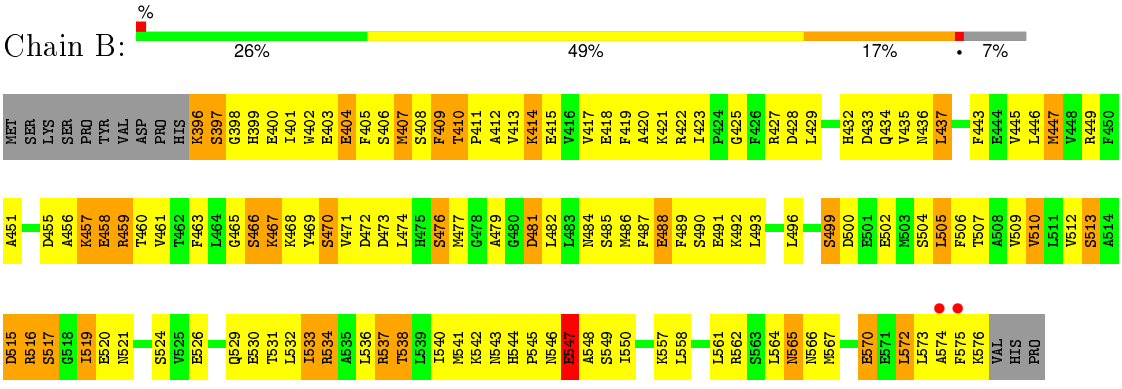
- Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

Chain A:



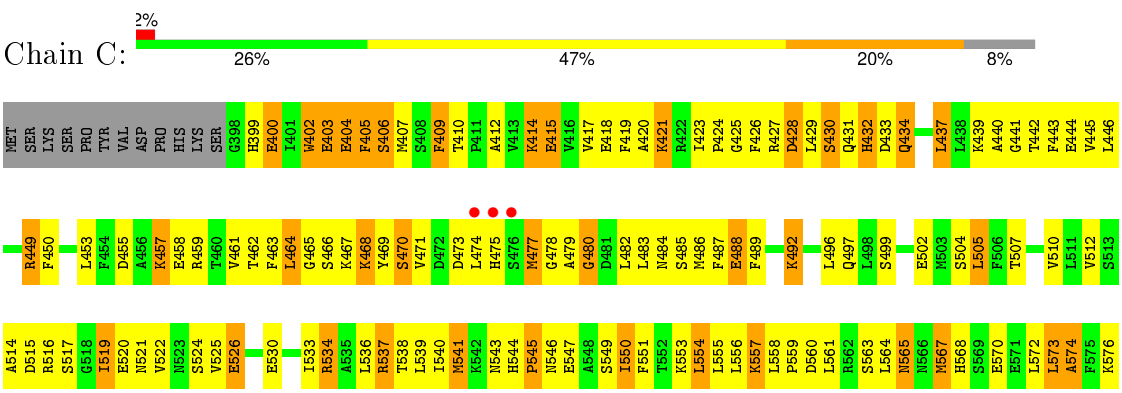
- Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

Chain B:



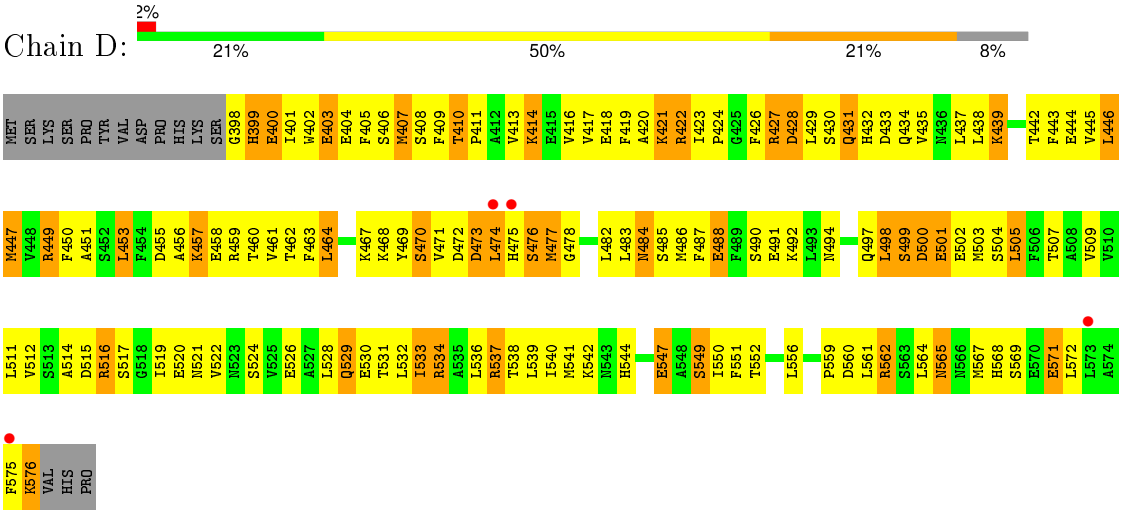
- Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

Chain C:



- Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	102.46Å 102.46Å 143.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.40 29.54 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.6 (99.00-2.40) 90.8 (29.54-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.29Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.138 , 0.220 0.141 , 0.139	Depositor DCC
R_{free} test set	1344 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 58.2	EDS
Estimated twinning fraction	0.096 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.096 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.097 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.096 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.487 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 30088 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5810	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.33	0/1460	0.97	3/1965 (0.2%)
1	B	0.39	0/1460	0.87	0/1965
1	C	0.33	0/1445	0.90	0/1946
1	D	0.38	0/1445	0.91	1/1946 (0.1%)
All	All	0.36	0/5810	0.91	4/7822 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	SER	CB-CA-C	10.55	130.14	110.10
1	A	409	PHE	N-CA-CB	-5.99	99.82	110.60
1	A	409	PHE	N-CA-C	5.95	127.07	111.00
1	D	562	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	410	THR	Peptide
1	A	475	HIS	Peptide
1	B	476	SER	Peptide
1	B	547	GLU	Peptide
1	C	567	MET	Peptide
1	D	464	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1436	0	1446	147	0
1	B	1436	0	1446	172	0
1	C	1421	0	1428	163	0
1	D	1421	0	1428	166	0
2	A	23	0	0	3	0
2	B	26	0	0	5	0
2	C	22	0	0	7	0
2	D	25	0	0	10	0
All	All	5810	0	5748	633	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 55.

All (633) 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:B:473:ASP:C	1:B:477:MET:HG2	1.47	1.33
1:B:473:ASP:O	1:B:477:MET:CG	1.80	1.28
1:A:470:SER:HB3	1:A:473:ASP:OD1	1.17	1.24
1:A:474:LEU:O	1:A:476:SER:O	1.67	1.13
1:B:473:ASP:O	1:B:476:SER:OG	1.66	1.13
1:B:473:ASP:HB3	1:B:477:MET:SD	1.89	1.13
1:D:534:ARG:HG3	1:D:534:ARG:HH11	1.03	1.10
1:A:410:THR:H	1:A:411:PRO:HD2	1.16	1.09
1:A:409:PHE:HA	1:A:412:ALA:HB3	1.13	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASP:O	1:B:477:MET:HG2	0.89	1.05
1:A:408:SER:O	1:A:411:PRO:HD2	1.59	1.03
1:C:463:PHE:HB2	1:C:467:LYS:HB2	1.05	1.01
1:A:402:TRP:O	1:A:406:SER:HB2	1.61	1.01
1:D:460:THR:HA	1:D:470:SER:HA	1.44	0.99
1:A:409:PHE:HA	1:A:412:ALA:CB	1.91	0.99
1:A:409:PHE:HD1	1:A:410:THR:N	1.60	0.98
1:B:473:ASP:C	1:B:477:MET:CG	2.25	0.97
1:A:470:SER:CB	1:A:473:ASP:OD1	2.13	0.95
1:B:404:GLU:HG2	1:B:467:LYS:HD2	1.48	0.95
1:B:473:ASP:CB	1:B:477:MET:SD	2.53	0.95
1:D:444:GLU:HG2	1:D:561:LEU:HB3	1.47	0.95
1:A:420:ALA:HA	1:A:423:ILE:HG13	1.49	0.93
1:A:398:GLY:HA2	1:A:477:MET:O	1.68	0.93
1:D:534:ARG:HH11	1:D:534:ARG:CG	1.81	0.93
1:B:471:VAL:HG12	1:B:474:LEU:HD12	1.50	0.92
1:A:410:THR:N	1:A:411:PRO:HD2	1.84	0.91
1:A:406:SER:OG	1:A:575:PHE:HE2	1.51	0.91
1:C:544:HIS:HB3	1:C:547:GLU:HB2	1.52	0.91
1:C:403:GLU:HA	1:C:406:SER:HB2	1.53	0.90
1:A:409:PHE:CD1	1:A:409:PHE:C	2.46	0.89
1:C:463:PHE:CB	1:C:467:LYS:HB2	1.99	0.89
1:D:413:VAL:HG13	1:D:442:THR:HG21	1.52	0.89
1:D:462:THR:HA	1:D:468:LYS:HA	1.55	0.88
1:B:516:ARG:HG3	1:B:516:ARG:HH11	1.37	0.87
1:A:409:PHE:HD1	1:A:409:PHE:C	1.78	0.86
1:B:474:LEU:O	1:B:477:MET:N	2.09	0.86
1:D:534:ARG:NH1	1:D:534:ARG:HG3	1.82	0.86
1:C:404:GLU:CG	1:C:467:LYS:HG3	2.08	0.84
1:B:471:VAL:HA	1:B:474:LEU:HG	1.60	0.83
1:A:406:SER:HB3	1:A:407:MET:HE3	1.60	0.82
1:C:463:PHE:HB2	1:C:467:LYS:CB	2.02	0.80
1:A:474:LEU:HD22	1:A:477:MET:CG	2.12	0.80
1:C:471:VAL:HG12	1:C:474:LEU:HD12	1.64	0.80
1:B:396:LYS:HD3	1:B:400:GLU:HG2	1.64	0.79
1:D:399:HIS:O	1:D:402:TRP:HB2	1.83	0.78
1:A:470:SER:HB3	1:A:473:ASP:CG	2.03	0.78
1:C:536:LEU:O	1:C:540:ILE:HG13	1.83	0.78
1:B:425:GLY:HA2	1:B:428:ASP:OD1	1.84	0.78
1:B:566:ASN:HB3	2:B:2024:HOH:O	1.83	0.78
1:B:401:ILE:HG13	1:B:469:TYR:CZ	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:O	1:D:421:LYS:HG2	1.85	0.77
1:A:403:GLU:O	1:A:407:MET:HG2	1.83	0.77
1:B:402:TRP:HE1	1:B:575:PHE:HZ	1.32	0.76
1:A:529:GLN:O	1:A:533:ILE:HB	1.86	0.76
1:A:474:LEU:HD22	1:A:477:MET:HG2	1.68	0.75
1:C:570:GLU:O	1:C:574:ALA:HB3	1.85	0.75
1:B:410:THR:HG21	1:B:576:LYS:HE2	1.68	0.75
1:C:402:TRP:HZ3	1:C:483:LEU:HD11	1.51	0.75
1:A:466:SER:HB2	1:C:431:GLN:HB2	1.69	0.75
1:D:449:ARG:HD2	2:D:2005:HOH:O	1.85	0.75
1:B:493:LEU:O	1:B:496:LEU:HB2	1.87	0.74
1:D:488:GLU:HB2	2:D:2014:HOH:O	1.88	0.74
1:A:397:SER:O	1:A:400:GLU:HB2	1.86	0.74
1:C:556:LEU:O	1:C:559:PRO:HD2	1.86	0.74
1:D:560:ASP:O	1:D:564:LEU:HG	1.87	0.73
1:A:516:ARG:O	1:A:519:ILE:HB	1.88	0.73
1:C:474:LEU:HD13	1:C:483:LEU:HB2	1.69	0.73
1:D:419:PHE:HA	1:D:422:ARG:HG3	1.69	0.73
1:A:544:HIS:HB3	1:A:547:GLU:HB2	1.70	0.73
1:C:404:GLU:CD	1:C:467:LYS:HG3	2.09	0.72
1:C:474:LEU:HD13	1:C:483:LEU:CB	2.19	0.72
1:C:553:LYS:O	1:C:557:LYS:HD3	1.89	0.72
1:C:425:GLY:HA2	1:C:428:ASP:OD1	1.89	0.72
1:B:515:ASP:OD1	1:B:517:SER:HB3	1.90	0.72
1:D:408:SER:O	1:D:411:PRO:HD2	1.91	0.71
1:C:402:TRP:HZ2	1:C:482:LEU:HD23	1.54	0.71
1:C:412:ALA:HA	1:C:415:GLU:OE2	1.90	0.71
1:C:540:ILE:HD11	1:C:554:LEU:HD12	1.73	0.71
1:B:398:GLY:HA3	1:B:477:MET:O	1.91	0.70
1:D:414:LYS:HD2	1:D:417:VAL:HG21	1.72	0.70
1:B:445:VAL:HG13	1:B:507:THR:HG23	1.73	0.70
1:D:482:LEU:HD22	1:D:568:HIS:HB3	1.73	0.70
1:C:402:TRP:CZ2	1:C:482:LEU:HD23	2.27	0.70
1:A:481:ASP:O	1:A:484:ASN:HB3	1.90	0.70
1:A:563:SER:O	1:A:567:MET:HB2	1.92	0.70
1:A:456:ALA:HB2	1:A:491:GLU:HB2	1.73	0.70
1:A:470:SER:O	1:A:473:ASP:OD2	2.09	0.70
1:B:447:MET:HG2	1:B:564:LEU:HD13	1.71	0.70
1:A:531:THR:O	1:A:534:ARG:HB2	1.92	0.69
1:B:396:LYS:N	1:B:400:GLU:HB3	2.06	0.69
1:C:462:THR:HG23	1:C:466:SER:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ASN:O	1:C:525:VAL:HG23	1.93	0.69
1:C:474:LEU:HD22	1:C:483:LEU:CD1	2.23	0.69
1:D:571:GLU:O	1:D:572:LEU:HD23	1.93	0.68
1:C:430:SER:O	1:C:434:GLN:HG3	1.93	0.68
1:A:401:ILE:HG12	1:A:474:LEU:HD11	1.76	0.68
1:B:546:ASN:O	1:C:573:LEU:HD22	1.94	0.68
1:C:492:LYS:O	1:C:496:LEU:HD13	1.95	0.67
1:D:544:HIS:HB3	1:D:547:GLU:HB2	1.77	0.67
1:A:403:GLU:O	1:A:407:MET:CG	2.43	0.67
1:D:414:LYS:HE2	1:D:417:VAL:HG11	1.77	0.66
1:D:499:SER:OG	1:D:501:GLU:HB2	1.95	0.66
1:A:401:ILE:HG12	1:A:474:LEU:CD1	2.24	0.66
1:A:455:ASP:OD2	1:A:457:LYS:HD3	1.95	0.66
1:A:443:PHE:HE1	1:A:572:LEU:HD12	1.61	0.66
1:C:462:THR:OG1	1:C:468:LYS:HG3	1.96	0.66
1:B:463:PHE:O	1:B:466:SER:N	2.29	0.66
1:B:403:GLU:HG2	1:B:407:MET:HE3	1.77	0.66
1:B:536:LEU:O	1:B:540:ILE:HG13	1.95	0.66
1:B:530:GLU:O	1:B:534:ARG:HG3	1.96	0.66
1:B:455:ASP:OD2	1:B:457:LYS:HB2	1.96	0.66
1:A:521:ASN:HB3	1:A:524:SER:OG	1.96	0.66
1:A:408:SER:O	1:A:410:THR:N	2.25	0.65
1:A:463:PHE:O	1:A:466:SER:N	2.23	0.65
1:C:455:ASP:OD2	1:C:457:LYS:HB2	1.97	0.65
1:C:471:VAL:HA	1:C:474:LEU:HB2	1.79	0.65
1:B:396:LYS:HD3	1:B:400:GLU:CG	2.26	0.65
1:A:410:THR:N	1:A:411:PRO:CD	2.60	0.65
1:A:473:ASP:OD2	1:A:474:LEU:N	2.30	0.65
1:B:546:ASN:CA	1:B:547:GLU:OE2	2.45	0.65
1:B:546:ASN:C	1:B:547:GLU:OE2	2.34	0.65
1:D:453:LEU:HD11	1:D:464:LEU:CD1	2.27	0.65
1:B:451:ALA:HA	1:B:490:SER:HB2	1.79	0.65
1:B:471:VAL:HG12	1:B:474:LEU:CD1	2.27	0.64
1:B:545:PRO:HD2	1:C:439:LYS:HE3	1.79	0.64
1:A:536:LEU:O	1:A:540:ILE:HD12	1.97	0.64
1:C:474:LEU:HD23	1:C:477:MET:SD	2.37	0.64
1:C:437:LEU:HD13	1:C:519:ILE:HD11	1.79	0.64
1:C:482:LEU:HD21	1:C:572:LEU:HD21	1.79	0.64
1:A:409:PHE:CD1	1:A:410:THR:N	2.53	0.64
1:A:418:GLU:O	1:A:421:LYS:HB2	1.98	0.64
1:C:474:LEU:HA	1:C:477:MET:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ARG:NE	1:D:427:ARG:H	1.95	0.64
1:D:516:ARG:HG2	1:D:522:VAL:HG13	1.79	0.63
1:D:423:ILE:HG22	1:D:426:PHE:HB2	1.80	0.63
1:C:463:PHE:O	1:C:466:SER:N	2.32	0.63
1:D:482:LEU:HD13	1:D:568:HIS:CD2	2.33	0.63
1:C:432:HIS:CD2	1:C:520:GLU:HG3	2.33	0.63
1:D:429:LEU:HB2	1:D:434:GLN:HG2	1.80	0.63
1:C:568:HIS:O	1:C:572:LEU:HG	1.98	0.63
1:D:471:VAL:HG11	1:D:487:PHE:CD1	2.34	0.63
1:B:404:GLU:HG3	1:B:463:PHE:HB2	1.79	0.62
1:B:505:LEU:HB3	1:B:536:LEU:HD13	1.81	0.62
1:C:554:LEU:O	1:C:557:LYS:HG2	1.98	0.62
1:A:559:PRO:HA	1:A:562:ARG:HB2	1.80	0.62
1:A:437:LEU:HD13	1:A:519:ILE:HD11	1.82	0.62
1:B:429:LEU:O	1:B:434:GLN:NE2	2.30	0.62
1:D:473:ASP:HB2	1:D:477:MET:SD	2.40	0.62
1:B:443:PHE:O	1:B:446:LEU:HB2	1.99	0.62
1:A:516:ARG:HA	1:A:519:ILE:HD13	1.80	0.62
1:A:526:GLU:HA	1:A:529:GLN:HG2	1.81	0.61
1:A:474:LEU:HA	1:A:477:MET:HB3	1.82	0.61
1:B:404:GLU:CG	1:B:467:LYS:HD2	2.28	0.61
1:C:414:LYS:HE2	1:C:418:GLU:OE1	1.99	0.61
1:D:565:ASN:HD22	1:D:569:SER:HB3	1.65	0.61
1:B:455:ASP:HB2	2:B:2011:HOH:O	2.00	0.61
1:C:516:ARG:HG2	1:C:522:VAL:HG13	1.83	0.61
1:B:471:VAL:HA	1:B:474:LEU:CG	2.28	0.61
1:B:403:GLU:O	1:B:406:SER:HB3	2.00	0.61
1:B:547:GLU:O	1:B:550:ILE:HG13	2.01	0.61
1:B:406:SER:HA	1:B:409:PHE:CE1	2.36	0.61
1:A:482:LEU:HD13	1:A:568:HIS:CD2	2.35	0.60
1:B:516:ARG:NH1	1:B:516:ARG:HG3	2.10	0.60
1:A:408:SER:O	1:A:411:PRO:CD	2.45	0.60
1:A:402:TRP:CZ2	1:A:572:LEU:HD21	2.36	0.60
1:D:568:HIS:HA	1:D:571:GLU:OE2	2.01	0.60
1:C:482:LEU:HD13	1:C:568:HIS:CD2	2.36	0.60
1:C:462:THR:CG2	1:C:466:SER:HA	2.31	0.60
1:C:419:PHE:CE2	1:C:423:ILE:HD11	2.36	0.60
1:B:458:GLU:HB3	1:B:460:THR:HG23	1.82	0.60
1:A:445:VAL:O	1:A:449:ARG:HB2	2.02	0.59
1:C:492:LYS:HE3	2:C:2013:HOH:O	2.02	0.59
1:B:489:PHE:CE1	1:B:557:LYS:HD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD22	1:B:479:ALA:HB3	1.84	0.59
1:B:408:SER:O	1:B:411:PRO:HD2	2.03	0.59
1:A:398:GLY:CA	1:A:477:MET:O	2.48	0.59
1:A:506:PHE:O	1:A:510:VAL:HG23	2.03	0.59
1:A:402:TRP:O	1:A:406:SER:CB	2.46	0.59
1:A:407:MET:O	1:A:408:SER:HB2	2.02	0.58
1:C:474:LEU:HD22	1:C:483:LEU:HD12	1.85	0.58
1:A:404:GLU:HA	1:A:404:GLU:OE1	2.00	0.58
1:B:458:GLU:HB3	1:B:460:THR:CG2	2.33	0.58
1:A:566:ASN:HB3	2:A:2023:HOH:O	2.03	0.58
1:B:482:LEU:O	1:B:486:MET:HG3	2.03	0.58
1:A:419:PHE:HA	1:A:422:ARG:NE	2.18	0.58
1:C:474:LEU:HD22	1:C:483:LEU:HD13	1.84	0.58
1:D:498:LEU:HD22	1:D:502:GLU:OE1	2.04	0.58
1:A:407:MET:O	1:A:408:SER:CB	2.51	0.58
1:B:397:SER:O	1:B:401:ILE:HD13	2.03	0.58
1:B:481:ASP:HA	1:B:484:ASN:HB3	1.84	0.58
1:B:473:ASP:HB2	1:B:477:MET:SD	2.39	0.58
1:B:536:LEU:HG	1:B:540:ILE:HD11	1.86	0.58
1:C:429:LEU:O	1:C:434:GLN:NE2	2.35	0.58
1:C:549:SER:O	1:C:553:LYS:HG3	2.03	0.58
1:B:403:GLU:O	1:B:407:MET:HG2	2.04	0.57
1:B:474:LEU:HA	1:B:477:MET:HB2	1.86	0.57
1:B:516:ARG:HA	1:B:519:ILE:HD13	1.84	0.57
1:A:431:GLN:O	1:A:435:VAL:HG23	2.04	0.57
1:D:534:ARG:NH1	1:D:534:ARG:CG	2.50	0.57
1:A:409:PHE:CE2	1:A:572:LEU:HD22	2.39	0.57
1:A:508:ALA:O	1:A:512:VAL:HG23	2.04	0.57
1:B:546:ASN:HB2	1:C:439:LYS:O	2.04	0.57
1:B:546:ASN:ND2	1:C:442:THR:HB	2.20	0.57
1:B:404:GLU:HG3	1:B:463:PHE:CB	2.34	0.57
1:A:529:GLN:HG3	1:A:530:GLU:N	2.20	0.57
1:C:484:ASN:O	1:C:488:GLU:HG2	2.05	0.57
1:B:474:LEU:N	1:B:477:MET:HG2	2.14	0.57
1:C:516:ARG:HG2	1:C:522:VAL:CG1	2.33	0.57
1:D:459:ARG:HB3	1:D:471:VAL:HG22	1.87	0.56
1:C:449:ARG:CZ	1:C:449:ARG:HB3	2.35	0.56
1:C:445:VAL:HG13	1:C:507:THR:HG23	1.87	0.56
1:C:461:VAL:HG12	1:C:469:TYR:HB2	1.88	0.56
1:D:420:ALA:HB1	1:D:426:PHE:CE2	2.40	0.56
1:A:474:LEU:O	1:A:477:MET:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:HB3	1:A:407:MET:CE	2.34	0.56
1:D:505:LEU:O	1:D:509:VAL:HG23	2.05	0.56
1:C:534:ARG:O	1:C:538:THR:HG23	2.05	0.56
1:D:529:GLN:O	1:D:533:ILE:HD12	2.05	0.56
1:A:454:PHE:CD2	1:A:461:VAL:HB	2.41	0.56
1:D:483:LEU:HA	1:D:486:MET:HB2	1.88	0.56
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.71	0.56
1:B:489:PHE:CZ	1:B:561:LEU:HD21	2.40	0.56
1:C:526:GLU:O	1:C:530:GLU:HB2	2.06	0.56
1:D:431:GLN:O	1:D:435:VAL:HG23	2.06	0.56
1:D:456:ALA:HB2	1:D:491:GLU:HG3	1.88	0.56
1:D:456:ALA:CB	1:D:491:GLU:HG3	2.36	0.55
1:A:429:LEU:O	1:A:434:GLN:NE2	2.33	0.55
1:A:410:THR:HA	1:A:413:VAL:HG23	1.87	0.55
1:D:423:ILE:CG2	1:D:426:PHE:HB2	2.35	0.55
1:D:429:LEU:O	1:D:434:GLN:NE2	2.30	0.55
1:C:404:GLU:CG	1:C:467:LYS:CG	2.84	0.55
1:D:537:ARG:HG3	1:D:551:PHE:CZ	2.42	0.55
1:C:471:VAL:HA	1:C:474:LEU:CG	2.37	0.55
1:D:502:GLU:HA	1:D:539:LEU:HD21	1.88	0.55
1:D:409:PHE:O	1:D:413:VAL:HG23	2.06	0.55
1:D:406:SER:HA	1:D:409:PHE:CZ	2.41	0.55
1:D:484:ASN:O	1:D:488:GLU:HG2	2.06	0.55
1:A:443:PHE:CD2	1:A:565:ASN:HA	2.42	0.55
1:C:430:SER:OG	1:C:432:HIS:HB3	2.06	0.55
1:A:443:PHE:CE2	1:A:565:ASN:HA	2.41	0.55
1:B:506:PHE:O	1:B:509:VAL:HB	2.07	0.55
1:A:482:LEU:HD22	1:A:568:HIS:HB3	1.89	0.55
1:C:576:LYS:HG2	1:C:576:LYS:O	2.07	0.55
1:B:485:SER:HA	1:B:488:GLU:HG3	1.88	0.55
1:C:563:SER:O	1:C:567:MET:HB2	2.07	0.54
1:B:443:PHE:HE1	1:B:572:LEU:HG	1.71	0.54
1:D:509:VAL:HG22	1:D:532:LEU:HB3	1.88	0.54
1:D:556:LEU:O	1:D:559:PRO:HD2	2.06	0.54
1:C:467:LYS:HB3	1:C:469:TYR:HE2	1.72	0.54
1:D:403:GLU:O	1:D:407:MET:HG2	2.07	0.54
1:D:521:ASN:HB3	1:D:524:SER:OG	2.07	0.54
1:C:482:LEU:CD2	1:C:572:LEU:HD21	2.38	0.54
1:D:446:LEU:O	1:D:450:PHE:HB2	2.08	0.54
1:B:469:TYR:O	1:B:470:SER:CB	2.56	0.54
1:D:414:LYS:HE2	1:D:417:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:LEU:HD11	1:D:464:LEU:HD12	1.90	0.54
1:B:474:LEU:C	1:B:477:MET:H	2.10	0.54
1:D:405:PHE:O	1:D:408:SER:HB2	2.07	0.54
1:A:474:LEU:HA	1:A:477:MET:CB	2.37	0.53
1:D:444:GLU:HB3	1:D:561:LEU:HD13	1.88	0.53
1:C:403:GLU:CA	1:C:406:SER:HB2	2.34	0.53
1:B:473:ASP:O	1:B:477:MET:SD	2.66	0.53
1:D:419:PHE:CA	1:D:422:ARG:HG3	2.35	0.53
1:B:401:ILE:O	1:B:401:ILE:CG2	2.56	0.53
1:A:409:PHE:HE2	1:A:572:LEU:HD22	1.73	0.53
1:C:474:LEU:HD13	1:C:483:LEU:HB3	1.90	0.53
1:D:443:PHE:O	1:D:447:MET:HE3	2.09	0.53
1:A:544:HIS:HB3	1:A:547:GLU:CB	2.39	0.53
1:B:546:ASN:N	1:B:547:GLU:OE2	2.42	0.53
1:C:557:LYS:O	1:C:561:LEU:HD12	2.08	0.53
1:B:549:SER:OG	1:C:574:ALA:HB1	2.09	0.53
1:D:430:SER:O	1:D:434:GLN:HG3	2.09	0.53
1:A:492:LYS:O	1:A:496:LEU:HD13	2.09	0.53
1:B:516:ARG:HA	1:B:519:ILE:CD1	2.38	0.52
1:B:546:ASN:HD22	1:C:442:THR:HB	1.74	0.52
1:A:540:ILE:O	1:A:544:HIS:HB2	2.09	0.52
1:D:462:THR:OG1	1:D:468:LYS:HG2	2.10	0.52
1:C:517:SER:HB3	2:C:2017:HOH:O	2.09	0.52
1:B:546:ASN:CB	1:B:547:GLU:OE2	2.58	0.52
1:C:541:MET:HA	2:C:2019:HOH:O	2.09	0.52
1:B:537:ARG:CZ	1:B:541:MET:HE1	2.39	0.52
1:B:471:VAL:O	1:B:474:LEU:HB2	2.09	0.52
1:B:443:PHE:CE2	1:B:565:ASN:HA	2.44	0.52
1:B:419:PHE:HA	1:B:422:ARG:CZ	2.40	0.52
1:C:482:LEU:HD11	1:C:486:MET:HE2	1.92	0.52
1:A:526:GLU:HG2	2:A:2015:HOH:O	2.10	0.52
1:C:432:HIS:CG	1:C:520:GLU:HG3	2.45	0.52
1:A:401:ILE:HG13	1:A:469:TYR:CZ	2.44	0.51
1:D:473:ASP:O	1:D:477:MET:N	2.34	0.51
1:C:405:PHE:HB3	1:C:409:PHE:CZ	2.45	0.51
1:A:411:PRO:O	1:A:415:GLU:OE2	2.29	0.51
1:B:474:LEU:HA	1:B:477:MET:CG	2.40	0.51
1:B:516:ARG:NH1	1:B:516:ARG:CG	2.71	0.51
1:D:536:LEU:O	1:D:540:ILE:HG13	2.09	0.51
1:A:516:ARG:HA	1:A:519:ILE:CD1	2.39	0.51
1:B:451:ALA:HA	1:B:490:SER:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:PHE:CE1	1:A:572:LEU:HD12	2.44	0.51
1:C:458:GLU:O	1:C:459:ARG:HB2	2.10	0.51
1:D:409:PHE:HB3	1:D:450:PHE:HE2	1.75	0.51
1:B:401:ILE:O	1:B:401:ILE:HG22	2.10	0.51
1:C:469:TYR:O	1:C:470:SER:HB2	2.10	0.51
1:B:443:PHE:CD2	1:B:565:ASN:HA	2.46	0.51
1:D:502:GLU:OE2	1:D:540:ILE:HA	2.11	0.51
1:A:482:LEU:HG	1:A:486:MET:HE3	1.93	0.51
1:C:444:GLU:HB2	1:C:510:VAL:HG11	1.92	0.51
1:B:404:GLU:HG2	1:B:467:LYS:CD	2.31	0.51
1:B:403:GLU:HG2	1:B:407:MET:CE	2.39	0.51
1:C:453:LEU:HB3	1:C:462:THR:O	2.10	0.50
1:D:445:VAL:HG13	1:D:507:THR:HG23	1.93	0.50
1:A:458:GLU:HB2	1:A:460:THR:HG23	1.93	0.50
1:D:476:SER:O	1:D:477:MET:C	2.49	0.50
1:A:406:SER:OG	1:A:575:PHE:CE2	2.39	0.50
1:C:540:ILE:CD1	1:C:554:LEU:HD12	2.40	0.50
1:B:411:PRO:O	1:B:415:GLU:OE2	2.28	0.50
1:B:558:LEU:HA	1:B:561:LEU:HD12	1.92	0.50
1:C:537:ARG:HG2	1:C:551:PHE:CZ	2.46	0.50
1:A:413:VAL:O	1:A:416:VAL:HB	2.12	0.50
1:B:512:VAL:HG12	1:B:529:GLN:HB3	1.94	0.50
1:B:432:HIS:O	1:B:436:ASN:OD1	2.30	0.50
1:D:515:ASP:OD1	1:D:517:SER:HB2	2.11	0.50
1:B:401:ILE:HG13	1:B:469:TYR:CE2	2.45	0.50
1:B:405:PHE:O	1:B:408:SER:HB2	2.11	0.50
1:D:432:HIS:CD2	1:D:520:GLU:HG3	2.46	0.50
1:C:459:ARG:O	1:C:471:VAL:HG22	2.11	0.50
1:B:411:PRO:HB2	2:B:2006:HOH:O	2.11	0.50
1:A:556:LEU:O	1:A:559:PRO:HD2	2.11	0.50
1:D:537:ARG:HG3	1:D:551:PHE:CE1	2.45	0.50
1:B:443:PHE:CE1	1:B:572:LEU:HG	2.46	0.50
1:C:484:ASN:O	1:C:487:PHE:HB3	2.11	0.50
1:D:509:VAL:CG2	1:D:532:LEU:HB3	2.42	0.50
1:A:406:SER:HG	1:A:575:PHE:HE2	0.69	0.50
1:C:471:VAL:HA	1:C:474:LEU:CB	2.42	0.50
1:D:419:PHE:CE2	1:D:507:THR:HG22	2.47	0.50
1:C:519:ILE:HG21	1:C:525:VAL:HG21	1.93	0.50
1:B:465:GLY:O	1:B:467:LYS:N	2.45	0.50
1:B:548:ALA:H	1:C:574:ALA:HB2	1.77	0.49
1:A:489:PHE:CZ	1:A:561:LEU:HD21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:CE2	1:A:434:GLN:HB3	2.47	0.49
1:D:494:ASN:HB2	2:D:2013:HOH:O	2.12	0.49
1:C:482:LEU:HD21	1:C:572:LEU:HD11	1.92	0.49
1:B:542:LYS:NZ	1:B:543:ASN:HD21	2.11	0.49
1:C:567:MET:HG2	1:C:568:HIS:CD2	2.46	0.49
1:D:427:ARG:H	1:D:427:ARG:CD	2.25	0.49
1:C:515:ASP:OD2	1:C:517:SER:HB2	2.11	0.49
1:C:505:LEU:HB3	1:C:536:LEU:HD13	1.95	0.49
1:A:396:LYS:N	1:A:400:GLU:HG2	2.27	0.49
1:B:505:LEU:O	1:B:509:VAL:HG23	2.11	0.49
1:D:459:ARG:HG2	1:D:487:PHE:CZ	2.47	0.49
1:A:406:SER:CB	1:A:407:MET:HE3	2.37	0.49
1:A:458:GLU:O	1:A:460:THR:HG22	2.13	0.49
1:B:414:LYS:HE2	1:B:418:GLU:HG2	1.95	0.49
1:C:474:LEU:CD2	1:C:483:LEU:HD13	2.42	0.49
1:C:560:ASP:O	1:C:564:LEU:HG	2.12	0.49
1:C:568:HIS:O	1:C:572:LEU:CD1	2.60	0.49
1:C:441:GLY:HA3	1:C:514:ALA:HB2	1.94	0.49
1:B:512:VAL:CG1	1:B:529:GLN:HB3	2.43	0.49
1:B:542:LYS:HZ2	1:B:543:ASN:HD21	1.60	0.49
1:D:550:ILE:HD11	2:D:2015:HOH:O	2.12	0.49
1:D:398:GLY:HA3	1:D:477:MET:O	2.12	0.49
1:B:461:VAL:HG13	1:B:461:VAL:O	2.13	0.49
1:A:408:SER:O	1:A:409:PHE:CD1	2.66	0.49
1:C:444:GLU:HB2	1:C:510:VAL:CG1	2.43	0.49
1:B:457:LYS:H	1:B:457:LYS:HD3	1.78	0.49
1:D:512:VAL:HG11	1:D:528:LEU:HG	1.94	0.48
1:A:475:HIS:CD2	1:A:484:ASN:HB2	2.48	0.48
1:C:399:HIS:CD2	2:C:2008:HOH:O	2.65	0.48
1:D:516:ARG:HA	1:D:519:ILE:HD12	1.96	0.48
1:B:512:VAL:HG21	1:B:532:LEU:HD12	1.95	0.48
1:A:443:PHE:CZ	1:A:447:MET:HE1	2.49	0.48
1:C:470:SER:O	1:C:474:LEU:HG	2.12	0.48
1:B:417:VAL:O	1:B:421:LYS:HG3	2.12	0.48
1:A:414:LYS:HD2	1:A:417:VAL:HB	1.95	0.48
1:B:465:GLY:O	1:B:467:LYS:HG3	2.14	0.48
1:A:412:ALA:O	1:A:415:GLU:HG2	2.13	0.48
1:A:512:VAL:HG11	1:A:528:LEU:HG	1.96	0.48
1:D:435:VAL:O	1:D:439:LYS:HB2	2.13	0.48
1:C:433:ASP:O	1:C:437:LEU:N	2.47	0.48
1:A:477:MET:HG3	1:A:477:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:SER:H	1:C:574:ALA:CB	2.26	0.48
1:A:474:LEU:HD22	1:A:477:MET:CB	2.43	0.47
1:A:450:PHE:O	1:A:453:LEU:HB2	2.14	0.47
1:D:499:SER:OG	1:D:501:GLU:CB	2.63	0.47
1:B:537:ARG:NH1	1:B:541:MET:HE1	2.29	0.47
1:D:416:VAL:HA	1:D:419:PHE:HB3	1.95	0.47
1:B:572:LEU:O	1:B:575:PHE:HD1	1.97	0.47
1:B:459:ARG:NH2	1:B:487:PHE:HE2	2.13	0.47
1:A:432:HIS:HD2	1:A:433:ASP:OD1	1.98	0.47
1:D:503:MET:HG2	2:D:2016:HOH:O	2.14	0.47
1:D:437:LEU:CD1	1:D:519:ILE:HD11	2.45	0.47
1:C:402:TRP:CZ3	1:C:483:LEU:HD21	2.50	0.47
1:D:463:PHE:HB2	1:D:467:LYS:HB2	1.97	0.47
1:B:549:SER:CB	1:C:574:ALA:HB1	2.44	0.47
1:A:396:LYS:N	1:A:400:GLU:HB3	2.29	0.47
1:A:433:ASP:O	1:A:437:LEU:HB2	2.15	0.47
1:A:528:LEU:O	1:A:532:LEU:HG	2.14	0.47
1:D:420:ALA:CB	1:D:438:LEU:HD21	2.45	0.47
1:B:474:LEU:N	1:B:477:MET:CG	2.75	0.47
1:D:538:THR:O	1:D:541:MET:HB2	2.15	0.47
1:B:396:LYS:HB2	1:B:400:GLU:CB	2.45	0.47
1:D:526:GLU:O	1:D:530:GLU:OE1	2.32	0.47
1:C:484:ASN:ND2	1:C:488:GLU:OE2	2.48	0.47
1:D:499:SER:HG	1:D:501:GLU:HB2	1.79	0.46
1:C:471:VAL:HA	1:C:474:LEU:HG	1.97	0.46
1:D:455:ASP:OD2	1:D:457:LYS:HB2	2.14	0.46
1:C:444:GLU:HB3	1:C:561:LEU:HB3	1.97	0.46
1:D:443:PHE:HE1	1:D:572:LEU:HD12	1.80	0.46
1:D:431:GLN:OE1	1:D:435:VAL:HG23	2.15	0.46
1:B:474:LEU:CA	1:B:477:MET:CG	2.93	0.46
1:B:471:VAL:O	1:B:474:LEU:N	2.48	0.46
1:A:410:THR:OG1	1:A:575:PHE:HB2	2.15	0.46
1:A:562:ARG:HA	1:A:562:ARG:HE	1.81	0.46
1:C:420:ALA:O	1:C:423:ILE:HB	2.15	0.46
1:C:463:PHE:O	1:C:465:GLY:N	2.48	0.46
1:D:455:ASP:CG	1:D:458:GLU:HG2	2.36	0.46
1:D:498:LEU:HD12	1:D:503:MET:CE	2.45	0.46
1:A:474:LEU:CA	1:A:477:MET:HB3	2.45	0.46
1:D:512:VAL:HG12	1:D:512:VAL:O	2.16	0.46
1:A:551:PHE:O	1:A:554:LEU:HB2	2.16	0.46
1:C:482:LEU:HD13	1:C:568:HIS:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:PRO:HB2	1:C:440:ALA:HA	1.97	0.46
1:D:407:MET:HG2	1:D:407:MET:H	1.47	0.46
1:D:473:ASP:O	1:D:477:MET:HG3	2.16	0.46
1:B:546:ASN:O	1:B:547:GLU:HG3	2.16	0.46
1:C:429:LEU:HB2	1:C:434:GLN:CG	2.45	0.46
1:A:474:LEU:HD13	1:A:477:MET:HG2	1.96	0.46
1:C:458:GLU:HA	1:C:458:GLU:OE1	2.16	0.46
1:C:420:ALA:HB1	1:C:426:PHE:CD2	2.51	0.46
1:C:544:HIS:HB3	1:C:547:GLU:CB	2.36	0.46
1:C:489:PHE:HE1	1:C:557:LYS:HB3	1.81	0.46
1:D:414:LYS:HD2	1:D:417:VAL:CG2	2.43	0.46
1:C:420:ALA:HB1	1:C:426:PHE:CE2	2.51	0.46
1:A:405:PHE:HB2	1:A:463:PHE:CE1	2.51	0.45
1:D:402:TRP:O	1:D:405:PHE:N	2.50	0.45
1:B:414:LYS:HD2	1:B:414:LYS:HA	1.46	0.45
1:A:419:PHE:HA	1:A:422:ARG:CZ	2.46	0.45
1:A:489:PHE:O	1:A:557:LYS:NZ	2.50	0.45
1:D:400:GLU:C	1:D:401:ILE:HD12	2.36	0.45
1:A:456:ALA:CB	1:A:491:GLU:HB2	2.43	0.45
1:B:538:THR:HA	1:B:541:MET:HB2	1.98	0.45
1:B:506:PHE:O	1:B:510:VAL:N	2.50	0.45
1:C:473:ASP:O	1:C:477:MET:N	2.50	0.45
1:C:478:GLY:O	1:C:480:GLY:N	2.50	0.45
1:D:534:ARG:O	1:D:538:THR:HG23	2.16	0.45
1:D:419:PHE:O	1:D:422:ARG:HG3	2.15	0.45
1:C:516:ARG:HA	1:C:519:ILE:CD1	2.46	0.45
1:D:427:ARG:NH2	1:D:428:ASP:OD1	2.50	0.45
1:B:506:PHE:O	1:B:509:VAL:N	2.50	0.45
1:B:544:HIS:N	1:B:545:PRO:HD3	2.31	0.45
1:B:481:ASP:N	1:B:481:ASP:OD2	2.50	0.45
1:C:484:ASN:HB2	2:C:2011:HOH:O	2.17	0.45
1:A:550:ILE:O	1:A:554:LEU:HG	2.17	0.45
1:C:474:LEU:CA	1:C:477:MET:HB2	2.47	0.45
1:D:561:LEU:O	1:D:564:LEU:HB2	2.17	0.45
1:D:445:VAL:HG21	1:D:511:LEU:HB2	1.98	0.45
1:D:492:LYS:NZ	2:D:2014:HOH:O	2.50	0.45
1:C:412:ALA:O	1:C:415:GLU:HG2	2.16	0.45
1:A:455:ASP:O	1:A:459:ARG:N	2.50	0.45
1:B:557:LYS:O	1:B:561:LEU:HG	2.16	0.45
1:D:474:LEU:O	1:D:475:HIS:C	2.54	0.45
1:C:568:HIS:O	1:C:572:LEU:CG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:PHE:O	1:B:446:LEU:N	2.50	0.45
1:B:509:VAL:O	1:B:513:SER:OG	2.30	0.45
1:B:529:GLN:HG3	1:B:530:GLU:N	2.31	0.45
1:B:489:PHE:O	1:B:557:LYS:NZ	2.50	0.45
1:B:432:HIS:CD2	1:B:520:GLU:HG3	2.52	0.45
1:D:424:PRO:HA	2:D:2003:HOH:O	2.17	0.45
1:B:409:PHE:O	1:B:412:ALA:HB3	2.16	0.45
1:C:482:LEU:O	1:C:486:MET:HG3	2.17	0.44
1:A:402:TRP:HZ3	1:A:483:LEU:HG	1.82	0.44
1:C:405:PHE:HB3	1:C:409:PHE:HZ	1.81	0.44
1:D:423:ILE:CD1	1:D:511:LEU:HD23	2.47	0.44
1:D:421:LYS:HG2	1:D:421:LYS:HZ3	1.69	0.44
1:B:482:LEU:HG	1:B:486:MET:CE	2.48	0.44
1:A:446:LEU:O	1:A:450:PHE:N	2.50	0.44
1:B:474:LEU:HA	1:B:474:LEU:HD23	1.85	0.44
1:A:573:LEU:O	1:A:575:PHE:N	2.49	0.44
1:D:413:VAL:HG13	1:D:442:THR:CG2	2.35	0.44
1:B:502:GLU:OE2	1:B:544:HIS:NE2	2.50	0.44
1:C:437:LEU:HD12	1:C:514:ALA:HB3	1.98	0.44
1:B:529:GLN:O	1:B:533:ILE:HB	2.17	0.44
1:D:451:ALA:HB1	1:D:490:SER:HA	2.00	0.44
1:B:414:LYS:NZ	1:B:418:GLU:OE1	2.48	0.44
1:C:502:GLU:HG2	1:C:539:LEU:HG	1.98	0.44
1:B:474:LEU:CA	1:B:477:MET:HG2	2.47	0.44
1:D:522:VAL:HG12	1:D:526:GLU:OE2	2.17	0.44
1:B:549:SER:H	1:C:574:ALA:HB1	1.83	0.44
1:D:565:ASN:ND2	2:D:2025:HOH:O	2.50	0.44
1:C:429:LEU:HB2	1:C:434:GLN:HG2	1.99	0.44
1:D:490:SER:O	1:D:494:ASN:OD1	2.34	0.44
1:D:409:PHE:HB3	1:D:450:PHE:CE2	2.53	0.44
1:B:499:SER:O	1:B:502:GLU:N	2.50	0.44
1:A:418:GLU:HA	1:A:421:LYS:HG3	1.99	0.44
1:C:417:VAL:HG12	1:C:418:GLU:OE1	2.17	0.44
1:B:489:PHE:HE1	1:B:557:LYS:HD2	1.81	0.44
1:A:566:ASN:ND2	2:A:2022:HOH:O	2.50	0.44
1:A:443:PHE:O	1:A:447:MET:HE2	2.17	0.44
1:C:463:PHE:O	1:C:464:LEU:C	2.55	0.44
1:D:460:THR:HG22	1:D:470:SER:HB2	1.98	0.44
1:C:405:PHE:O	1:C:409:PHE:CE1	2.71	0.44
1:B:502:GLU:CD	1:B:544:HIS:HE2	2.21	0.44
1:D:428:ASP:N	1:D:428:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LYS:HG2	1:C:421:LYS:H	1.50	0.44
1:D:455:ASP:OD2	1:D:458:GLU:N	2.50	0.44
1:C:496:LEU:HD23	1:C:554:LEU:HD23	2.00	0.44
1:B:408:SER:O	1:B:412:ALA:HB2	2.18	0.44
1:A:408:SER:C	1:A:411:PRO:HD2	2.35	0.44
1:D:467:LYS:O	1:D:469:TYR:HD2	2.01	0.44
1:D:482:LEU:HD22	1:D:568:HIS:CB	2.46	0.44
1:B:420:ALA:HA	1:B:423:ILE:HD12	2.00	0.44
1:D:455:ASP:OD2	1:D:457:LYS:N	2.50	0.43
1:D:469:TYR:HB3	1:D:470:SER:H	1.55	0.43
1:D:414:LYS:NZ	1:D:418:GLU:OE1	2.50	0.43
1:B:412:ALA:O	1:B:415:GLU:HG2	2.18	0.43
1:C:414:LYS:O	1:C:414:LYS:HD2	2.18	0.43
1:D:537:ARG:HG3	1:D:551:PHE:CE2	2.53	0.43
1:D:482:LEU:HG	1:D:486:MET:CE	2.48	0.43
1:D:427:ARG:HE	1:D:427:ARG:H	1.62	0.43
1:D:458:GLU:HB2	1:D:460:THR:OG1	2.18	0.43
1:C:546:ASN:N	1:C:547:GLU:OE2	2.50	0.43
1:D:413:VAL:HG22	1:D:446:LEU:HD11	1.99	0.43
1:D:572:LEU:O	1:D:575:PHE:CD1	2.71	0.43
1:B:456:ALA:HB1	1:B:491:GLU:OE2	2.19	0.43
1:D:399:HIS:HB2	1:D:478:GLY:O	2.18	0.43
1:D:414:LYS:HE2	1:D:417:VAL:CB	2.49	0.43
1:C:512:VAL:HG12	1:C:512:VAL:O	2.18	0.43
1:A:482:LEU:HD21	1:A:572:LEU:HD11	2.01	0.43
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.74	0.43
1:C:510:VAL:HG21	1:C:561:LEU:HD13	2.00	0.43
1:B:540:ILE:HG23	1:B:544:HIS:CD2	2.54	0.43
1:A:433:ASP:O	1:A:437:LEU:N	2.50	0.43
1:C:516:ARG:HA	1:C:519:ILE:HD13	1.99	0.43
1:B:414:LYS:CE	1:B:418:GLU:OE1	2.67	0.43
1:C:443:PHE:CE2	1:C:565:ASN:HA	2.54	0.43
1:D:414:LYS:HA	1:D:417:VAL:HG23	2.01	0.43
1:A:543:ASN:C	1:A:545:PRO:HD3	2.39	0.43
1:A:443:PHE:CE1	1:A:447:MET:HE1	2.53	0.43
1:B:414:LYS:HE3	1:B:417:VAL:HB	1.99	0.43
1:B:433:ASP:O	1:B:437:LEU:HD22	2.19	0.43
1:B:410:THR:HG21	1:B:576:LYS:CE	2.43	0.43
1:B:410:THR:HG22	1:B:411:PRO:N	2.34	0.43
1:D:484:ASN:HB2	2:D:2012:HOH:O	2.17	0.43
1:C:415:GLU:HG2	1:C:415:GLU:H	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASP:OD2	1:A:458:GLU:N	2.50	0.43
1:A:557:LYS:O	1:A:560:ASP:HB2	2.19	0.43
1:D:576:LYS:HE3	1:D:576:LYS:HB3	1.55	0.43
1:A:401:ILE:HG13	1:A:469:TYR:CE1	2.53	0.43
1:B:402:TRP:NE1	1:B:575:PHE:HZ	2.07	0.43
1:A:475:HIS:NE2	1:A:481:ASP:OD2	2.52	0.43
1:A:484:ASN:O	1:A:487:PHE:N	2.50	0.43
1:A:562:ARG:HA	1:A:562:ARG:NE	2.34	0.43
1:D:549:SER:O	1:D:552:THR:N	2.52	0.43
1:D:437:LEU:HD21	1:D:512:VAL:HA	2.01	0.42
1:A:405:PHE:CE1	1:A:409:PHE:HD2	2.37	0.42
1:C:568:HIS:O	1:C:572:LEU:HD12	2.19	0.42
1:B:409:PHE:O	1:B:413:VAL:HG23	2.19	0.42
1:A:455:ASP:CG	1:A:457:LYS:HD3	2.38	0.42
1:B:482:LEU:HG	1:B:486:MET:HE3	2.01	0.42
1:D:564:LEU:HD23	1:D:564:LEU:N	2.34	0.42
1:D:443:PHE:CE2	1:D:565:ASN:HA	2.54	0.42
1:A:401:ILE:HG12	1:A:474:LEU:HD13	1.98	0.42
1:C:399:HIS:HD2	2:C:2008:HOH:O	1.99	0.42
1:D:547:GLU:O	1:D:550:ILE:HG13	2.19	0.42
1:B:474:LEU:HD22	1:B:479:ALA:CB	2.49	0.42
1:D:453:LEU:HD11	1:D:464:LEU:HD11	2.00	0.42
1:D:537:ARG:HE	1:D:537:ARG:HB3	1.64	0.42
1:D:474:LEU:HD23	1:D:474:LEU:N	2.34	0.42
1:A:574:ALA:O	1:A:575:PHE:HD1	2.03	0.42
1:C:558:LEU:HB2	1:C:559:PRO:HD3	2.01	0.42
1:D:433:ASP:O	1:D:437:LEU:HB2	2.19	0.42
1:D:530:GLU:O	1:D:534:ARG:HB2	2.20	0.42
1:A:460:THR:O	1:A:460:THR:OG1	2.30	0.42
1:C:543:ASN:C	1:C:545:PRO:HD3	2.40	0.42
1:C:446:LEU:O	1:C:450:PHE:CD1	2.72	0.42
1:B:403:GLU:OE2	1:B:407:MET:HE1	2.20	0.42
1:B:543:ASN:C	1:B:545:PRO:HD3	2.40	0.42
1:C:459:ARG:NH1	1:C:459:ARG:HG2	2.35	0.41
1:C:576:LYS:HB3	1:C:576:LYS:HE2	1.82	0.41
1:C:404:GLU:OE1	1:C:467:LYS:HG3	2.19	0.41
1:D:467:LYS:O	1:D:469:TYR:CD2	2.73	0.41
1:D:406:SER:HA	1:D:409:PHE:CE1	2.54	0.41
1:B:445:VAL:HG13	1:B:507:THR:CG2	2.43	0.41
1:B:447:MET:CG	1:B:564:LEU:HD13	2.47	0.41
1:A:559:PRO:O	1:A:562:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:GLY:O	1:C:466:SER:C	2.58	0.41
1:C:475:HIS:CD2	2:C:2011:HOH:O	2.73	0.41
1:B:421:LYS:NZ	1:D:472:ASP:OD1	2.47	0.41
1:B:399:HIS:HE1	2:B:2003:HOH:O	2.03	0.41
1:C:402:TRP:O	1:C:405:PHE:HB2	2.21	0.41
1:D:438:LEU:O	1:D:442:THR:OG1	2.30	0.41
1:C:547:GLU:HB3	1:C:550:ILE:HG13	2.02	0.41
1:B:417:VAL:HG12	1:B:421:LYS:NZ	2.36	0.41
1:B:421:LYS:HD3	1:D:472:ASP:HB3	2.02	0.41
1:A:543:ASN:O	1:A:545:PRO:HD3	2.21	0.41
1:D:500:ASP:OD1	1:D:500:ASP:N	2.52	0.41
1:C:409:PHE:CE2	1:C:572:LEU:HD22	2.56	0.41
1:D:410:THR:HG22	1:D:411:PRO:N	2.35	0.41
1:D:423:ILE:HA	1:D:424:PRO:HD3	1.72	0.41
1:B:515:ASP:HB3	2:B:2017:HOH:O	2.19	0.41
1:C:455:ASP:O	1:C:459:ARG:N	2.50	0.41
1:C:459:ARG:HH11	1:C:459:ARG:HG2	1.86	0.41
1:D:405:PHE:CD2	1:D:409:PHE:HE2	2.37	0.41
1:B:402:TRP:O	1:B:406:SER:HB2	2.20	0.41
1:B:507:THR:O	1:B:510:VAL:HB	2.21	0.41
1:A:455:ASP:OD2	1:A:458:GLU:HG2	2.20	0.41
1:B:557:LYS:HD3	1:B:557:LYS:HA	1.90	0.41
1:D:505:LEU:HD23	1:D:505:LEU:HA	1.75	0.41
1:D:537:ARG:HA	1:D:551:PHE:CD2	2.55	0.41
1:B:521:ASN:O	1:B:524:SER:OG	2.33	0.41
1:D:514:ALA:HB2	2:D:2004:HOH:O	2.20	0.41
1:D:437:LEU:HD12	1:D:519:ILE:HD11	2.03	0.41
1:D:455:ASP:OD1	1:D:458:GLU:HG2	2.21	0.41
1:D:461:VAL:O	1:D:469:TYR:N	2.54	0.41
1:D:418:GLU:O	1:D:421:LYS:HB2	2.21	0.41
1:A:405:PHE:CZ	1:A:409:PHE:HD2	2.39	0.40
1:A:572:LEU:HD23	1:A:572:LEU:HA	1.85	0.40
1:C:404:GLU:HG2	1:C:467:LYS:CG	2.51	0.40
1:C:555:LEU:O	1:C:558:LEU:HG	2.21	0.40
1:D:502:GLU:CA	1:D:539:LEU:HD21	2.51	0.40
1:B:570:GLU:O	1:B:574:ALA:HB3	2.21	0.40
1:D:413:VAL:CG2	1:D:446:LEU:HD11	2.52	0.40
1:B:546:ASN:HB3	1:C:573:LEU:HD22	2.03	0.40
1:D:572:LEU:O	1:D:575:PHE:HD1	2.04	0.40
1:C:449:ARG:NH1	1:C:450:PHE:HE1	2.19	0.40
1:B:474:LEU:HA	1:B:477:MET:CB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ASP:O	1:C:477:MET:HB2	2.21	0.40
1:D:516:ARG:HG3	1:D:516:ARG:NH1	2.36	0.40
1:D:414:LYS:HE2	1:D:417:VAL:HB	2.04	0.40
1:C:443:PHE:CD2	1:C:565:ASN:HA	2.55	0.40
1:A:564:LEU:HA	1:A:564:LEU:HD23	1.98	0.40
1:A:474:LEU:HD22	1:A:477:MET:SD	2.60	0.40
1:D:488:GLU:O	1:D:492:LYS:HG3	2.22	0.40
1:C:430:SER:HG	1:C:432:HIS:HB3	1.86	0.40
1:C:423:ILE:HA	1:C:424:PRO:HD3	1.85	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	179/194 (92%)	146 (82%)	28 (16%)	5 (3%)	6 5
1	B	179/194 (92%)	154 (86%)	21 (12%)	4 (2%)	8 9
1	C	177/194 (91%)	142 (80%)	26 (15%)	9 (5%)	2 1
1	D	177/194 (91%)	146 (82%)	29 (16%)	2 (1%)	17 25
All	All	712/776 (92%)	588 (83%)	104 (15%)	20 (3%)	6 5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLY
1	A	408	SER
1	A	409	PHE
1	B	470	SER
1	A	470	SER
1	A	480	GLY

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Mol	Chain	Res	Type
1	C	464	LEU
1	C	470	SER
1	C	480	GLY
1	C	400	GLU
1	B	466	SER
1	C	432	HIS
1	C	434	GLN
1	D	477	MET
1	C	479	ALA
1	C	574	ALA
1	D	457	LYS
1	B	467	LYS
1	B	547	GLU
1	C	545	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	161/174 (92%)	115 (71%)	46 (29%)	0	0
1	B	161/174 (92%)	119 (74%)	42 (26%)	0	0
1	C	159/174 (91%)	120 (76%)	39 (24%)	1	1
1	D	159/174 (91%)	114 (72%)	45 (28%)	0	0
All	All	640/696 (92%)	468 (73%)	172 (27%)	0	0

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	LYS
1	A	397	SER
1	A	399	HIS
1	A	400	GLU
1	A	402	TRP
1	A	404	GLU
1	A	407	MET

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Mol	Chain	Res	Type
1	A	409	PHE
1	A	414	LYS
1	A	415	GLU
1	A	422	ARG
1	A	427	ARG
1	A	430	SER
1	A	435	VAL
1	A	447	MET
1	A	449	ARG
1	A	457	LYS
1	A	460	THR
1	A	464	LEU
1	A	466	SER
1	A	468	LYS
1	A	474	LEU
1	A	475	HIS
1	A	481	ASP
1	A	482	LEU
1	A	485	SER
1	A	488	GLU
1	A	491	GLU
1	A	497	GLN
1	A	500	ASP
1	A	504	SER
1	A	505	LEU
1	A	519	ILE
1	A	520	GLU
1	A	525	VAL
1	A	533	ILE
1	A	537	ARG
1	A	538	THR
1	A	552	THR
1	A	563	SER
1	A	565	ASN
1	A	567	MET
1	A	569	SER
1	A	571	GLU
1	A	573	LEU
1	A	576	LYS
1	B	396	LYS
1	B	397	SER
1	B	404	GLU

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Mol	Chain	Res	Type
1	B	407	MET
1	B	409	PHE
1	B	410	THR
1	B	414	LYS
1	B	427	ARG
1	B	435	VAL
1	B	437	LEU
1	B	447	MET
1	B	449	ARG
1	B	457	LYS
1	B	458	GLU
1	B	459	ARG
1	B	468	LYS
1	B	472	ASP
1	B	481	ASP
1	B	488	GLU
1	B	492	LYS
1	B	499	SER
1	B	500	ASP
1	B	504	SER
1	B	505	LEU
1	B	510	VAL
1	B	513	SER
1	B	515	ASP
1	B	516	ARG
1	B	517	SER
1	B	519	ILE
1	B	526	GLU
1	B	531	THR
1	B	533	ILE
1	B	534	ARG
1	B	537	ARG
1	B	538	THR
1	B	562	ARG
1	B	565	ASN
1	B	567	MET
1	B	570	GLU
1	B	572	LEU
1	B	573	LEU
1	C	400	GLU
1	C	402	TRP
1	C	403	GLU

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Mol	Chain	Res	Type
1	C	404	GLU
1	C	405	PHE
1	C	406	SER
1	C	407	MET
1	C	409	PHE
1	C	410	THR
1	C	414	LYS
1	C	415	GLU
1	C	421	LYS
1	C	427	ARG
1	C	428	ASP
1	C	430	SER
1	C	437	LEU
1	C	449	ARG
1	C	457	LYS
1	C	468	LYS
1	C	477	MET
1	C	485	SER
1	C	488	GLU
1	C	492	LYS
1	C	497	GLN
1	C	499	SER
1	C	504	SER
1	C	505	LEU
1	C	519	ILE
1	C	524	SER
1	C	526	GLU
1	C	533	ILE
1	C	534	ARG
1	C	537	ARG
1	C	541	MET
1	C	550	ILE
1	C	554	LEU
1	C	557	LYS
1	C	565	ASN
1	C	573	LEU
1	D	399	HIS
1	D	400	GLU
1	D	403	GLU
1	D	404	GLU
1	D	407	MET
1	D	410	THR

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Mol	Chain	Res	Type
1	D	414	LYS
1	D	421	LYS
1	D	422	ARG
1	D	427	ARG
1	D	428	ASP
1	D	431	GLN
1	D	439	LYS
1	D	446	LEU
1	D	447	MET
1	D	449	ARG
1	D	453	LEU
1	D	470	SER
1	D	473	ASP
1	D	474	LEU
1	D	476	SER
1	D	484	ASN
1	D	485	SER
1	D	488	GLU
1	D	497	GLN
1	D	498	LEU
1	D	499	SER
1	D	500	ASP
1	D	501	GLU
1	D	504	SER
1	D	505	LEU
1	D	516	ARG
1	D	529	GLN
1	D	531	THR
1	D	533	ILE
1	D	534	ARG
1	D	537	ARG
1	D	542	LYS
1	D	547	GLU
1	D	549	SER
1	D	562	ARG
1	D	565	ASN
1	D	567	MET
1	D	571	GLU
1	D	576	LYS

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

Mol	Chain	Res	Type
1	A	484	ASN
1	A	565	ASN
1	A	566	ASN
1	A	568	HIS
1	B	436	ASN
1	B	543	ASN
1	B	546	ASN
1	B	565	ASN
1	C	399	HIS
1	C	431	GLN
1	C	432	HIS
1	C	484	ASN
1	C	565	ASN
1	D	432	HIS
1	D	484	ASN
1	D	565	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	181/194 (93%)	-1.01	2 (1%)	82	82	9, 28, 89, 135	0
1	B	181/194 (93%)	-0.97	2 (1%)	82	82	8, 30, 97, 129	0
1	C	179/194 (92%)	-0.96	3 (1%)	73	72	5, 29, 81, 122	0
1	D	179/194 (92%)	-0.87	4 (2%)	65	64	7, 35, 115, 138	0
All	All	720/776 (92%)	-0.95	11 (1%)	76	75	5, 31, 94, 138	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	474	LEU	12.1
1	D	475	HIS	4.2
1	D	474	LEU	3.4
1	C	475	HIS	3.2
1	D	575	PHE	2.9
1	B	575	PHE	2.9
1	B	574	ALA	2.7
1	A	475	HIS	2.6
1	D	573	LEU	2.2
1	A	401	ILE	2.1
1	C	476	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.