Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:41 AM EDT

PDB ID	:	4N0F
Title	:	Human FcRn complexed with human serum albumin
Authors	:	Oganesyan, V.; Wu, H.; Dall'Acqua, W.F.
Deposited on	:	2013-10-01
Resolution	:	3.02 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:

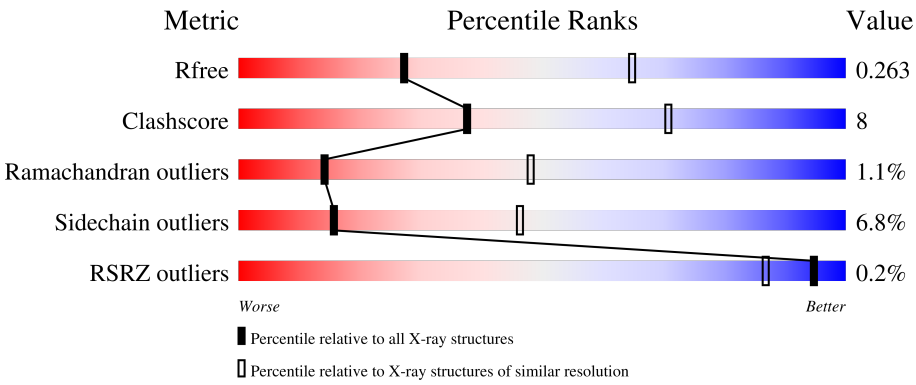
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	271	77% 18% • •
1	E	271	74% 20% • •
1	H	271	73% 20% • •
1	K	271	76% 18% • •
2	B	99	82% 16% •

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Mol	Chain	Length	Quality of chain
2	F	99	78% 21% •
2	I	99	% 88% 11% •
2	L	99	86% 12% •
3	D	585	80% 17% •
3	G	585	78% 19% •
3	J	585	78% 19% •
3	M	585	81% 16% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30181 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2079	1330	360	381	8	0	0	0
1	E	264	2079	1330	360	381	8	0	0	0
1	H	264	2079	1330	360	381	8	0	0	0
1	K	264	2079	1330	360	381	8	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	828	528	140	157	3	0	0	0
2	F	99	828	528	140	157	3	0	0	0
2	I	99	828	528	140	157	3	0	0	0
2	L	99	829	528	140	158	3	0	0	0

- Molecule 3 is a protein called Serum albumin.

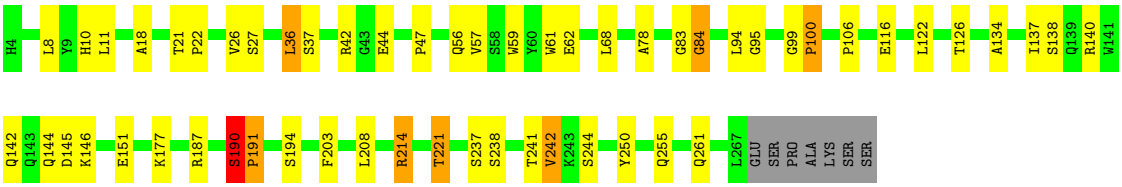
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	583	4638	2929	784	884	41	0	0	0
3	G	583	4638	2929	784	884	41	0	0	0
3	J	583	4638	2929	784	884	41	0	0	0
3	M	583	4638	2929	784	884	41	0	0	0

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.

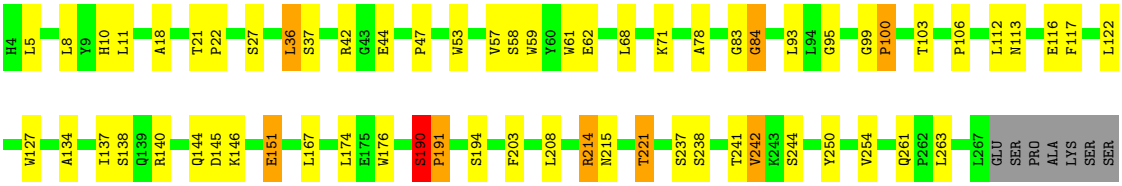
• Molecule 1: IgG receptor FcRn large subunit p51

Chain A:



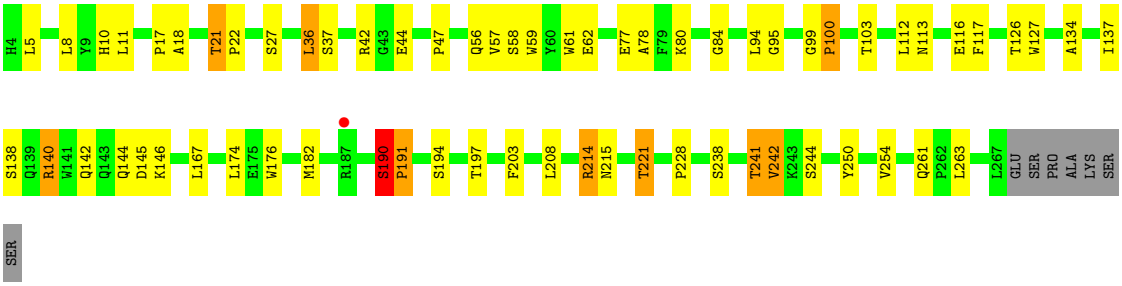
• Molecule 1: IgG receptor FcRn large subunit p51

Chain E:



• Molecule 1: IgG receptor FcRn large subunit p51

Chain H:



• Molecule 1: IgG receptor FcRn large subunit p51

Chain K:

H4 L5 L8 Y9 H10 L11 A18 T21 P22 S27 Q33 L36 S37 E44 P47 W53 V57 S58 W59 Y60 W61 E62 K71 A78 G83 G84 L93 L94 G95 G99 P100 D101 N102 T103 E116 F117 T126 W127 A134 I137 S138

Q139 R140 W141 Q142 Q143 Q144 D145 K146 L174 K177 S190 P191 S194 T197 F203 L208 R214 T221 S237 S238 T241 V242 K243 S244 Y250 Q261 L267 GLU SER PRO ALA LYS SER SER

- Molecule 2: Beta-2-microglobulin

Chain B: 82% 16% •

I1 Q2 N24 S33 V37 D38 L39 L40 R45 L65 Y66 F70 E74 N83 H84 V85 K94 W95 D96 M99

- Molecule 2: Beta-2-microglobulin

Chain F: 78% 21% •

I1 Q2 I7 Q8 V9 N24 V27 S33 D34 V37 E44 E47 L65 Y66 F70 E74 V82 N83 H84 V85 S88 Q89 K94 M99

- Molecule 2: Beta-2-microglobulin

Chain I: % 88% 11% •

I1 Q2 S33 V37 Y66 F70 T73 E74 N83 H84 V85 K94 M99

- Molecule 2: Beta-2-microglobulin

Chain L: 86% 12% •

I1 N24 S33 V37 L65 Y66 F70 E74 N83 H84 Q89 P90 K94 M99

- Molecule 3: Serum albumin

Chain D: 80% 17% •

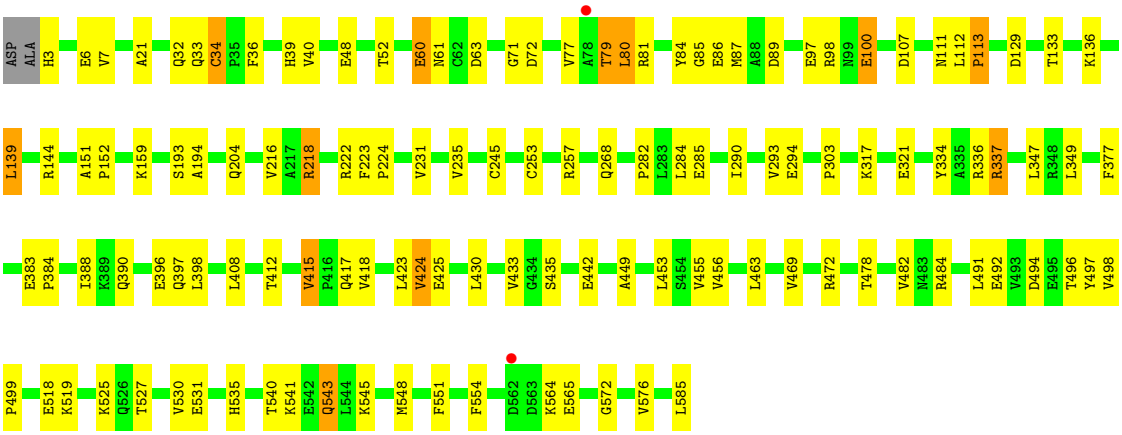
ASP ALA H3 E6 Q32 Q33 C34 H39 L42 V43 N44 E45 V46 T47 E48 T52 C53 V54 E60 N61 C62 D63 G71 D72 K73 T76 V77 A78 T79 L80 R81 Y84 G85 E86 M87 A88 D89 A92 E97 R98 N99 E100 L103 D107 N111 L112

P113 D129 T133 F134 L135 K136 L139 R144 A151 P152 K162 A172 S193 A194 K212 A213 W214 A215 V216 A217 R218 R222 F223 P224 V235 C245 C253 R257 Q268 K281 P282 L283 E292 V293 E294 P303 K317 E321 Y334

A335 R336 R337 V343 L347 E383 P384 Q390 E396 T412 V415 P416 Q417 V418 T422 L423 V426 L430 V433 G434 S435 E442 V455 V456 L463 V469 V482 N483 R484 D494 E495 T496 Y497 V498 P499 E518 K519 Q526 V530 E531

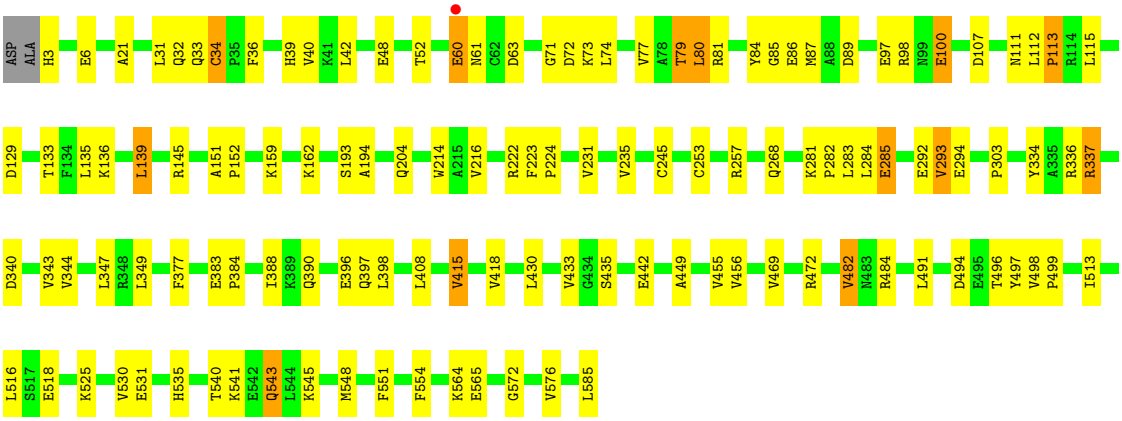
• Molecule 3: Serum albumin

Chain G:



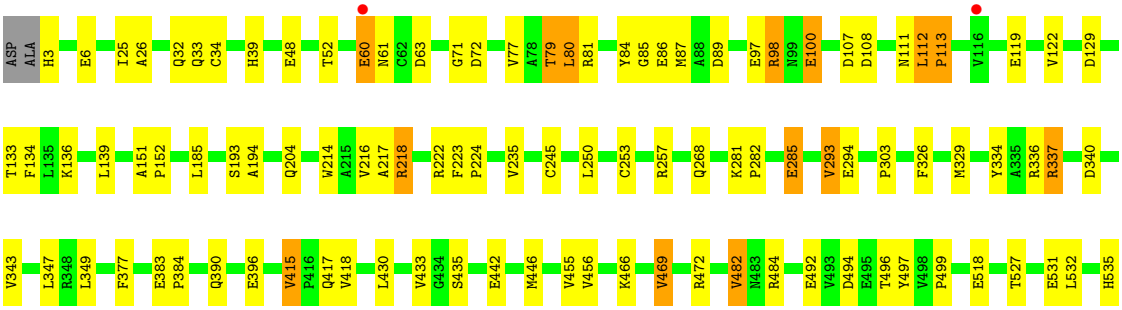
• Molecule 3: Serum albumin

Chain J:



• Molecule 3: Serum albumin

Chain M:



T540
Q543
V547
F551
F554
K564
E565
L575
L585

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.47Å 115.92Å 186.24Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	20.00 – 3.02 44.26 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.02) 99.2 (44.26-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.260 0.228 , 0.263	Depositor DCC
R_{free} test set	5501 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	30181	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2461e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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)

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	0.79	1/2145 (0.0%)	0.81	0/2915
1	E	0.80	3/2145 (0.1%)	0.81	0/2915
1	H	0.79	2/2145 (0.1%)	0.79	1/2915 (0.0%)
1	K	0.80	1/2145 (0.0%)	0.78	0/2915
2	B	0.72	1/851 (0.1%)	0.76	1/1152 (0.1%)
2	F	0.68	0/851	0.73	0/1152
2	I	0.63	0/851	0.71	0/1152
2	L	0.65	0/852	0.69	0/1152
3	D	0.63	0/4728	0.77	1/6377 (0.0%)
3	G	0.65	0/4728	0.77	1/6377 (0.0%)
3	J	0.63	0/4728	0.76	1/6377 (0.0%)
3	M	0.62	0/4728	0.77	4/6377 (0.1%)
All	All	0.69	8/30897 (0.0%)	0.77	9/41776 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	151	GLU	CD-OE2	6.67	1.32	1.25
1	A	151	GLU	CD-OE2	6.43	1.32	1.25
1	H	127	TRP	CD2-CE2	5.40	1.47	1.41
1	H	176	TRP	CD2-CE2	5.29	1.47	1.41
2	B	95	TRP	CD2-CE2	5.28	1.47	1.41
1	E	127	TRP	CD2-CE2	5.05	1.47	1.41
1	K	127	TRP	CD2-CE2	5.02	1.47	1.41
1	E	176	TRP	CD2-CE2	5.00	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	340	ASP	CB-CG-OD2	7.52	125.07	118.30
2	B	45	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	H	190	SER	CB-CA-C	5.77	121.06	110.10
3	M	63	ASP	CB-CG-OD2	5.68	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	63	ASP	CB-CG-OD1	-5.56	113.29	118.30
3	G	218	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	M	218	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	D	218	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	M	340	ASP	CB-CG-OD1	5.06	122.85	118.30

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	2079	0	1990	40	0
1	E	2079	0	1990	41	0
1	H	2079	0	1990	51	0
1	K	2079	0	1990	39	0
2	B	828	0	794	8	0
2	F	828	0	794	8	0
2	I	828	0	794	7	0
2	L	829	0	794	6	0
3	D	4638	0	4563	75	0
3	G	4638	0	4563	75	0
3	J	4638	0	4563	78	0
3	M	4638	0	4563	63	0
All	All	30181	0	29388	459	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 8.

All (459) 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)
3:D:33:GLN:HE21	3:D:112:LEU:CD1	1.59	1.16
3:M:112:LEU:HD23	3:M:113:PRO:HD2	1.29	1.08
3:J:33:GLN:HE21	3:J:112:LEU:CD1	1.71	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:CD1	1:A:94:LEU:HD13	1.91	1.00
3:D:33:GLN:HE21	3:D:112:LEU:HD11	1.29	0.97
3:J:33:GLN:NE2	3:J:112:LEU:HD11	1.79	0.96
3:J:33:GLN:HE21	3:J:112:LEU:HD11	1.30	0.96
3:J:115:LEU:HB2	3:J:145:ARG:HH12	1.28	0.95
1:A:11:LEU:HD13	1:A:94:LEU:HD13	1.50	0.94
3:G:430:LEU:HD23	3:G:456:VAL:HG11	1.54	0.87
3:J:33:GLN:NE2	3:J:112:LEU:CD1	2.35	0.87
1:A:57:VAL:HG11	3:D:111:ASN:HB3	1.58	0.84
3:M:112:LEU:HD23	3:M:113:PRO:CD	2.08	0.83
3:D:430:LEU:HD23	3:D:456:VAL:HG11	1.58	0.83
3:D:33:GLN:NE2	3:D:112:LEU:CD1	2.41	0.82
3:J:115:LEU:CB	3:J:145:ARG:HH12	1.93	0.81
3:G:33:GLN:HE21	3:G:112:LEU:CD1	1.93	0.81
2:B:83:ASN:HD22	2:B:84:HIS:H	1.27	0.79
3:M:151:ALA:HB3	3:M:152:PRO:HD3	1.65	0.78
2:L:83:ASN:HD22	2:L:84:HIS:H	1.32	0.75
1:A:36:LEU:HD23	1:A:37:SER:N	2.02	0.74
1:A:44:GLU:HG3	3:D:417:GLN:NE2	2.03	0.74
3:J:151:ALA:HB3	3:J:152:PRO:HD3	1.70	0.74
1:H:8:LEU:HD23	1:H:95:GLY:HA3	1.68	0.74
3:J:194:ALA:HB1	3:J:455:VAL:CG1	2.17	0.74
1:K:144:GLN:O	1:K:146:LYS:N	2.21	0.74
3:J:77:VAL:O	3:J:80:LEU:HG	1.89	0.73
3:D:33:GLN:HE21	3:D:112:LEU:HD12	1.51	0.73
3:G:151:ALA:HB3	3:G:152:PRO:HD3	1.69	0.73
3:J:115:LEU:HB2	3:J:145:ARG:NH1	2.03	0.73
3:D:77:VAL:O	3:D:80:LEU:HG	1.89	0.73
3:M:77:VAL:O	3:M:80:LEU:HG	1.89	0.72
3:D:151:ALA:HB3	3:D:152:PRO:HD3	1.72	0.72
1:E:144:GLN:O	1:E:146:LYS:N	2.22	0.72
1:A:144:GLN:O	1:A:146:LYS:N	2.22	0.72
1:A:18:ALA:O	1:A:21:THR:HB	1.91	0.70
3:J:430:LEU:HD23	3:J:456:VAL:HG11	1.72	0.70
3:G:430:LEU:CD2	3:G:456:VAL:HG11	2.22	0.69
3:G:77:VAL:O	3:G:80:LEU:HG	1.92	0.69
2:L:83:ASN:HD22	2:L:84:HIS:N	1.89	0.69
1:H:78:ALA:HB1	1:H:137:ILE:HD13	1.73	0.69
3:D:33:GLN:NE2	3:D:112:LEU:HD11	2.06	0.68
1:H:144:GLN:O	1:H:146:LYS:N	2.23	0.68
2:I:2:GLN:HE22	2:I:85:VAL:HG11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:ASN:HD22	2:I:84:HIS:H	1.40	0.67
3:M:194:ALA:HB1	3:M:455:VAL:CG1	2.24	0.67
3:J:33:GLN:HE21	3:J:112:LEU:HD13	1.55	0.67
1:E:18:ALA:O	1:E:21:THR:HB	1.95	0.66
3:G:33:GLN:NE2	3:G:112:LEU:CD1	2.58	0.66
1:H:18:ALA:O	1:H:21:THR:HB	1.96	0.66
1:K:18:ALA:O	1:K:21:THR:HB	1.96	0.66
1:A:11:LEU:HD13	1:A:94:LEU:CD1	2.25	0.66
1:E:241:THR:O	1:E:242:VAL:HG23	1.97	0.65
3:M:430:LEU:HD23	3:M:456:VAL:HG11	1.78	0.65
1:H:11:LEU:HD12	1:H:11:LEU:H	1.61	0.65
2:B:83:ASN:HD22	2:B:84:HIS:N	1.95	0.65
1:A:36:LEU:HD23	1:A:36:LEU:C	2.17	0.65
1:K:57:VAL:HG11	3:M:111:ASN:HB3	1.78	0.64
1:E:36:LEU:HD23	1:E:37:SER:N	2.12	0.64
3:M:81:ARG:NH2	3:M:89:ASP:OD2	2.31	0.64
1:K:36:LEU:HD23	1:K:37:SER:N	2.12	0.64
3:G:36:PHE:O	3:G:40:VAL:HG23	1.97	0.63
3:D:216:VAL:HG22	3:D:235:VAL:HG21	1.80	0.63
3:J:81:ARG:NH2	3:J:89:ASP:OD2	2.31	0.63
3:D:33:GLN:NE2	3:D:112:LEU:HD12	2.12	0.63
1:E:57:VAL:HG11	3:G:111:ASN:HB3	1.80	0.63
1:E:57:VAL:HG11	3:G:111:ASN:CG	2.19	0.62
3:J:415:VAL:O	3:J:415:VAL:CG1	2.48	0.62
3:G:540:THR:H	3:G:543:GLN:HE21	1.48	0.62
1:K:44:GLU:CD	3:M:469:VAL:HG22	2.20	0.62
3:D:430:LEU:CD2	3:D:456:VAL:HG11	2.30	0.62
3:D:81:ARG:NH2	3:D:89:ASP:OD2	2.32	0.62
3:D:415:VAL:CG1	3:D:415:VAL:O	2.48	0.62
3:M:347:LEU:HB2	3:M:482:VAL:HG21	1.82	0.62
3:J:415:VAL:HG13	3:J:418:VAL:HG23	1.82	0.62
1:K:47:PRO:HB3	1:K:61:TRP:CZ2	2.35	0.62
3:G:81:ARG:NH2	3:G:89:ASP:OD2	2.32	0.61
3:M:79:THR:O	3:M:81:ARG:N	2.34	0.61
1:H:47:PRO:HB3	1:H:61:TRP:CZ2	2.36	0.61
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.83	0.61
3:J:34:CYS:N	3:J:84:TYR:OH	2.34	0.61
3:G:415:VAL:HG13	3:G:418:VAL:HG23	1.82	0.61
3:G:347:LEU:HB2	3:G:482:VAL:HG21	1.83	0.61
1:H:11:LEU:CD1	1:H:94:LEU:HD12	2.29	0.61
3:J:540:THR:H	3:J:543:GLN:HE21	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:MET:CE	1:H:254:VAL:HB	2.31	0.60
1:K:57:VAL:HG11	3:M:111:ASN:CB	2.30	0.60
3:M:415:VAL:CG1	3:M:415:VAL:O	2.50	0.60
1:E:11:LEU:HD12	1:E:11:LEU:H	1.66	0.60
3:M:34:CYS:N	3:M:84:TYR:OH	2.35	0.60
3:D:79:THR:O	3:D:81:ARG:N	2.34	0.59
3:J:541:LYS:NZ	3:J:545:LYS:HE3	2.17	0.59
3:D:540:THR:H	3:D:543:GLN:HE21	1.51	0.59
3:J:216:VAL:CG2	3:J:235:VAL:HG21	2.32	0.59
3:J:216:VAL:HG22	3:J:235:VAL:HG21	1.84	0.59
1:E:57:VAL:HG11	3:G:111:ASN:CB	2.32	0.59
3:J:79:THR:O	3:J:81:ARG:N	2.36	0.59
2:F:83:ASN:HD22	2:F:84:HIS:H	1.49	0.59
1:K:93:LEU:O	1:K:94:LEU:HD23	2.02	0.59
1:A:57:VAL:HG11	3:D:111:ASN:CB	2.30	0.58
3:D:60:GLU:O	3:D:61:ASN:HB2	2.02	0.58
1:E:47:PRO:HB3	1:E:61:TRP:CZ2	2.38	0.58
1:K:11:LEU:H	1:K:11:LEU:HD12	1.68	0.58
3:J:194:ALA:HB1	3:J:455:VAL:HG11	1.84	0.58
3:M:194:ALA:HB1	3:M:455:VAL:HG13	1.86	0.58
1:E:21:THR:HG23	1:E:22:PRO:HD2	1.86	0.58
3:G:79:THR:O	3:G:81:ARG:N	2.36	0.58
3:G:33:GLN:NE2	3:G:112:LEU:HD11	2.18	0.58
3:G:34:CYS:N	3:G:84:TYR:OH	2.36	0.58
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.39	0.58
3:D:34:CYS:N	3:D:84:TYR:OH	2.35	0.58
3:G:218:ARG:HH11	3:G:218:ARG:HG2	1.69	0.58
1:H:36:LEU:HD23	1:H:37:SER:N	2.18	0.58
3:D:218:ARG:HG2	3:D:218:ARG:HH11	1.69	0.57
1:H:182:MET:HE2	1:H:254:VAL:HG11	1.85	0.57
3:J:194:ALA:HB1	3:J:455:VAL:HG13	1.84	0.57
3:G:541:LYS:HZ2	3:G:545:LYS:HE3	1.68	0.57
1:E:78:ALA:HB1	1:E:137:ILE:HD13	1.86	0.57
3:D:293:VAL:HG22	3:D:294:GLU:H	1.69	0.57
3:M:60:GLU:O	3:M:61:ASN:HB2	2.05	0.57
3:M:218:ARG:HG2	3:M:218:ARG:HH11	1.68	0.56
3:G:531:GLU:O	3:G:535:HIS:HD2	1.88	0.56
1:K:57:VAL:HG12	1:K:58:SER:O	2.05	0.56
2:I:2:GLN:HE22	2:I:85:VAL:CG1	2.18	0.56
1:E:71:LYS:NZ	1:E:151:GLU:OE1	2.28	0.56
3:D:415:VAL:HG13	3:D:418:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:VAL:HG11	3:J:111:ASN:HB3	1.87	0.56
1:E:57:VAL:HG12	1:E:58:SER:N	2.21	0.56
1:H:11:LEU:HD11	1:H:94:LEU:HD12	1.88	0.56
1:K:33:GLN:NE2	1:K:174:LEU:HD23	2.20	0.56
3:J:80:LEU:O	3:J:84:TYR:N	2.39	0.55
3:J:159:LYS:CE	3:J:284:LEU:HD12	2.36	0.55
3:G:216:VAL:HG22	3:G:235:VAL:HG21	1.87	0.55
3:G:388:ILE:HD13	3:G:449:ALA:CB	2.36	0.55
3:M:80:LEU:O	3:M:84:TYR:N	2.40	0.55
3:D:417:GLN:HA	3:D:417:GLN:OE1	2.05	0.55
1:K:214:ARG:HG3	1:K:250:TYR:CZ	2.42	0.55
3:G:33:GLN:HE21	3:G:112:LEU:HD11	1.69	0.55
3:J:293:VAL:HG22	3:J:294:GLU:H	1.71	0.54
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.89	0.54
3:M:531:GLU:O	3:M:535:HIS:HD2	1.90	0.54
3:D:80:LEU:O	3:D:84:TYR:N	2.40	0.54
3:G:60:GLU:O	3:G:61:ASN:HB2	2.07	0.54
3:J:347:LEU:HB2	3:J:482:VAL:HG21	1.89	0.54
1:K:190:SER:OG	1:K:191:PRO:HD2	2.08	0.54
3:D:347:LEU:HB2	3:D:482:VAL:HG21	1.88	0.54
3:G:541:LYS:NZ	3:G:545:LYS:HE3	2.23	0.54
1:K:21:THR:HG23	1:K:22:PRO:HD2	1.89	0.54
1:A:203:PHE:CZ	1:A:208:LEU:HD13	2.43	0.54
2:F:2:GLN:NE2	2:F:85:VAL:HG11	2.23	0.54
1:H:182:MET:HE2	1:H:254:VAL:CG1	2.38	0.54
3:D:531:GLU:O	3:D:535:HIS:HD2	1.91	0.53
3:J:48:GLU:O	3:J:52:THR:HG23	2.07	0.53
1:A:190:SER:OG	1:A:191:PRO:HD2	2.09	0.53
3:J:60:GLU:O	3:J:61:ASN:HB2	2.08	0.53
1:E:190:SER:OG	1:E:191:PRO:HD2	2.08	0.53
1:K:208:LEU:C	1:K:208:LEU:HD23	2.29	0.53
1:A:21:THR:HG23	1:A:22:PRO:HD2	1.91	0.53
3:G:80:LEU:O	3:G:84:TYR:N	2.40	0.53
3:D:214:TRP:CD1	3:D:343:VAL:HG11	2.44	0.53
3:G:194:ALA:HB1	3:G:455:VAL:CG1	2.38	0.53
1:E:134:ALA:O	1:E:138:SER:HB2	2.09	0.53
1:H:190:SER:OG	1:H:191:PRO:HD2	2.09	0.53
1:H:221:THR:HG22	1:H:238:SER:OG	2.08	0.53
3:M:48:GLU:O	3:M:52:THR:HG23	2.07	0.53
3:M:282:PRO:HG2	3:M:285:GLU:HG3	1.91	0.53
3:D:112:LEU:HD21	3:D:144:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:282:PRO:HG2	3:J:285:GLU:HG3	1.91	0.52
3:G:424:VAL:HG12	3:G:425:GLU:N	2.23	0.52
3:G:159:LYS:HE2	3:G:284:LEU:HD12	1.91	0.52
1:A:134:ALA:O	1:A:138:SER:HB2	2.10	0.52
3:J:531:GLU:O	3:J:535:HIS:HD2	1.93	0.52
2:L:37:VAL:HB	2:L:66:TYR:CE1	2.45	0.52
3:M:224:PRO:O	3:M:336:ARG:NH1	2.42	0.52
1:H:182:MET:HE2	1:H:254:VAL:HB	1.92	0.52
1:E:36:LEU:HD23	1:E:36:LEU:C	2.31	0.51
1:K:134:ALA:O	1:K:138:SER:HB2	2.10	0.51
3:J:224:PRO:O	3:J:336:ARG:NH1	2.43	0.51
3:M:216:VAL:HG22	3:M:235:VAL:HG21	1.92	0.51
3:G:282:PRO:HG2	3:G:285:GLU:HG3	1.92	0.51
3:G:415:VAL:HG13	3:G:418:VAL:CG2	2.40	0.51
1:H:134:ALA:O	1:H:138:SER:HB2	2.10	0.51
1:K:221:THR:HG22	1:K:238:SER:OG	2.10	0.51
1:A:214:ARG:HG3	1:A:250:TYR:CZ	2.46	0.51
1:A:241:THR:O	1:A:242:VAL:HG23	2.11	0.51
3:J:388:ILE:HD13	3:J:449:ALA:CB	2.39	0.51
3:M:216:VAL:CG2	3:M:235:VAL:HG21	2.41	0.51
3:D:99:ASN:HD21	3:D:103:LEU:HD11	1.76	0.51
2:I:37:VAL:HB	2:I:66:TYR:CE1	2.46	0.51
3:D:224:PRO:O	3:D:336:ARG:NH1	2.44	0.51
3:J:383:GLU:HB3	3:J:384:PRO:HD3	1.93	0.51
3:M:383:GLU:HB3	3:M:384:PRO:HD3	1.93	0.51
3:J:231:VAL:O	3:J:235:VAL:HG23	2.11	0.51
3:G:408:LEU:HD11	3:G:530:VAL:CG2	2.41	0.50
1:H:36:LEU:HD23	1:H:36:LEU:C	2.31	0.50
3:D:415:VAL:HG13	3:D:418:VAL:CG2	2.41	0.50
2:F:37:VAL:HB	2:F:66:TYR:CE1	2.46	0.50
3:G:48:GLU:O	3:G:52:THR:HG23	2.12	0.50
3:G:224:PRO:O	3:G:336:ARG:NH1	2.44	0.50
1:H:190:SER:CB	1:H:191:PRO:CD	2.89	0.50
1:K:203:PHE:CZ	1:K:208:LEU:HD13	2.47	0.50
3:M:108:ASP:OD1	3:M:466:LYS:NZ	2.44	0.50
3:D:415:VAL:O	3:D:415:VAL:HG13	2.11	0.50
1:H:182:MET:HE2	1:H:254:VAL:CB	2.40	0.50
3:M:293:VAL:HG22	3:M:294:GLU:H	1.76	0.50
1:H:11:LEU:HD13	1:H:94:LEU:HD12	1.94	0.50
1:A:8:LEU:HD23	1:A:95:GLY:HA3	1.92	0.50
3:G:159:LYS:CE	3:G:284:LEU:HD12	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:GLN:HE22	3:D:107:ASP:H	1.60	0.49
3:J:303:PRO:O	3:J:337:ARG:NH1	2.45	0.49
1:K:36:LEU:HD23	1:K:36:LEU:C	2.33	0.49
1:A:221:THR:HG22	1:A:238:SER:OG	2.12	0.49
2:I:2:GLN:NE2	2:I:85:VAL:HG11	2.27	0.49
1:A:11:LEU:CD1	1:A:94:LEU:CD1	2.77	0.49
3:G:397:GLN:O	3:G:398:LEU:HD23	2.12	0.49
3:M:540:THR:H	3:M:543:GLN:HE21	1.60	0.49
3:M:303:PRO:O	3:M:337:ARG:NH1	2.45	0.49
3:G:383:GLU:HB3	3:G:384:PRO:HD3	1.94	0.49
1:H:182:MET:HE1	1:H:254:VAL:HG21	1.93	0.49
3:J:36:PHE:O	3:J:40:VAL:HG23	2.12	0.49
1:A:59:TRP:NE1	3:D:463:LEU:HD13	2.28	0.49
3:D:303:PRO:O	3:D:337:ARG:NH1	2.46	0.49
3:J:159:LYS:HE2	3:J:284:LEU:HD12	1.95	0.49
1:H:167:LEU:HD23	1:H:174:LEU:CD1	2.42	0.49
3:D:383:GLU:HB3	3:D:384:PRO:HD3	1.94	0.48
1:E:208:LEU:HD23	1:E:208:LEU:C	2.33	0.48
3:J:135:LEU:HD21	3:J:162:LYS:HB2	1.95	0.48
1:E:203:PHE:CE2	1:E:208:LEU:HD13	2.48	0.48
1:H:57:VAL:HG11	3:J:111:ASN:CB	2.42	0.48
3:J:71:GLY:O	3:J:72:ASP:C	2.51	0.48
1:H:214:ARG:HG3	1:H:250:TYR:CZ	2.49	0.48
2:I:83:ASN:HD22	2:I:84:HIS:N	2.08	0.48
3:J:32:GLN:HE22	3:J:107:ASP:H	1.62	0.48
3:G:112:LEU:HD21	3:G:144:ARG:NH1	2.28	0.48
3:M:71:GLY:O	3:M:72:ASP:C	2.52	0.48
3:J:21:ALA:HB1	3:J:139:LEU:HD21	1.95	0.48
1:K:57:VAL:HG12	1:K:58:SER:N	2.28	0.48
1:K:203:PHE:CE2	1:K:208:LEU:HD13	2.48	0.48
1:E:214:ARG:NH1	1:E:215:ASN:HD22	2.11	0.48
3:G:303:PRO:O	3:G:337:ARG:NH1	2.46	0.48
1:H:197:THR:HG21	2:I:99:MET:HG2	1.96	0.48
1:E:214:ARG:HG3	1:E:250:TYR:CZ	2.49	0.48
1:H:214:ARG:NH1	1:H:215:ASN:HD22	2.12	0.48
1:K:44:GLU:OE1	3:M:469:VAL:HG22	2.14	0.48
1:K:241:THR:O	1:K:242:VAL:HG23	2.14	0.48
3:D:216:VAL:CG2	3:D:235:VAL:HG21	2.44	0.48
3:G:518:GLU:OE1	3:G:518:GLU:HA	2.14	0.48
3:M:494:ASP:OD1	3:M:496:THR:HB	2.14	0.48
3:D:71:GLY:O	3:D:72:ASP:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:VAL:HG11	3:J:111:ASN:CG	2.34	0.47
1:A:208:LEU:C	1:A:208:LEU:HD23	2.35	0.47
3:J:85:GLY:O	3:J:87:MET:N	2.47	0.47
3:G:71:GLY:O	3:G:72:ASP:C	2.52	0.47
1:H:182:MET:HE1	1:H:254:VAL:CG2	2.43	0.47
1:K:57:VAL:HG11	3:M:111:ASN:CG	2.34	0.47
3:M:518:GLU:HA	3:M:518:GLU:OE1	2.13	0.47
3:D:99:ASN:ND2	3:D:103:LEU:HD11	2.28	0.47
3:J:31:LEU:HG	3:J:74:LEU:HD22	1.96	0.47
3:J:415:VAL:HG13	3:J:418:VAL:CG2	2.43	0.47
1:H:78:ALA:HB1	1:H:137:ILE:CD1	2.44	0.47
1:H:182:MET:CE	1:H:254:VAL:CB	2.92	0.47
1:K:8:LEU:HD23	1:K:95:GLY:HA3	1.95	0.47
3:M:34:CYS:HB3	3:M:39:HIS:NE2	2.30	0.47
3:M:85:GLY:O	3:M:87:MET:N	2.47	0.47
1:E:254:VAL:CG1	1:E:263:LEU:HB3	2.45	0.47
1:H:77:GLU:HG2	1:H:140:ARG:NH1	2.30	0.47
1:K:44:GLU:OE2	3:M:469:VAL:HG22	2.15	0.47
3:D:194:ALA:HB1	3:D:455:VAL:CG1	2.44	0.47
1:E:99:GLY:N	1:E:103:THR:O	2.44	0.47
1:E:203:PHE:CZ	1:E:208:LEU:HD13	2.50	0.47
3:G:293:VAL:HG22	3:G:294:GLU:H	1.80	0.47
1:H:254:VAL:O	1:H:254:VAL:HG13	2.14	0.47
3:J:214:TRP:CD1	3:J:343:VAL:HG11	2.49	0.47
3:J:494:ASP:OD1	3:J:496:THR:HB	2.15	0.47
3:D:48:GLU:O	3:D:52:THR:HG23	2.15	0.47
3:D:518:GLU:OE1	3:D:518:GLU:HA	2.15	0.47
1:H:80:LYS:HD2	1:H:140:ARG:HH12	1.80	0.47
3:G:194:ALA:HB1	3:G:455:VAL:HG13	1.97	0.47
3:J:513:ILE:HG22	3:J:516:LEU:HD11	1.97	0.46
3:D:34:CYS:HB3	3:D:39:HIS:NE2	2.31	0.46
3:J:518:GLU:HA	3:J:518:GLU:OE1	2.14	0.46
3:M:223:PHE:N	3:M:224:PRO:CD	2.79	0.46
3:J:223:PHE:N	3:J:224:PRO:CD	2.79	0.46
1:K:53:TRP:CZ3	3:M:527:THR:HG22	2.51	0.46
3:G:85:GLY:O	3:G:87:MET:N	2.48	0.46
3:G:472:ARG:NH2	3:G:492:GLU:O	2.49	0.46
1:K:93:LEU:C	1:K:94:LEU:HD23	2.36	0.46
2:B:2:GLN:NE2	2:B:85:VAL:HG11	2.31	0.46
3:D:42:LEU:O	3:D:46:VAL:HG23	2.16	0.46
1:K:99:GLY:O	1:K:100:PRO:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:572:GLY:O	3:G:576:VAL:HG23	2.15	0.45
1:E:221:THR:HG22	1:E:238:SER:OG	2.16	0.45
1:H:17:PRO:HB2	1:H:21:THR:HG22	1.99	0.45
3:J:541:LYS:HZ2	3:J:545:LYS:HE3	1.82	0.45
1:A:187:ARG:NH1	2:B:96:ASP:OD1	2.49	0.45
3:D:422:THR:O	3:D:426:VAL:HG23	2.16	0.45
1:E:93:LEU:HD12	1:E:93:LEU:HA	1.73	0.45
3:G:494:ASP:OD1	3:G:496:THR:HB	2.16	0.45
3:D:73:LYS:O	3:D:76:THR:HB	2.17	0.45
2:F:34:ASP:O	2:F:84:HIS:HD2	2.00	0.45
3:G:33:GLN:HE21	3:G:112:LEU:HD13	1.76	0.45
3:M:185:LEU:HA	3:M:185:LEU:HD12	1.61	0.45
1:A:56:GLN:NE2	1:A:57:VAL:H	2.15	0.45
1:H:112:LEU:HD12	1:H:113:ASN:H	1.82	0.45
1:H:242:VAL:HG22	1:H:250:TYR:CZ	2.51	0.45
1:E:42:ARG:NH1	3:G:498:VAL:O	2.50	0.45
3:G:223:PHE:N	3:G:224:PRO:CD	2.79	0.45
3:D:194:ALA:HB1	3:D:455:VAL:HG13	1.99	0.45
1:E:59:TRP:NE1	3:G:463:LEU:HD13	2.32	0.45
1:A:56:GLN:HE21	1:A:57:VAL:H	1.64	0.44
3:D:99:ASN:O	3:D:103:LEU:HD12	2.16	0.44
3:D:223:PHE:N	3:D:224:PRO:CD	2.79	0.44
1:H:99:GLY:O	1:H:100:PRO:C	2.56	0.44
1:A:99:GLY:O	1:A:100:PRO:C	2.55	0.44
3:D:85:GLY:O	3:D:87:MET:N	2.50	0.44
1:E:57:VAL:CG1	1:E:58:SER:N	2.80	0.44
3:G:349:LEU:HD22	3:G:377:PHE:CG	2.52	0.44
1:K:57:VAL:CG1	1:K:58:SER:N	2.80	0.44
3:M:112:LEU:O	3:M:113:PRO:C	2.55	0.44
3:J:281:LYS:HB3	3:J:282:PRO:HD2	2.00	0.44
3:D:54:VAL:HG12	2:F:88:SER:HB3	1.99	0.44
1:H:11:LEU:HD12	1:H:11:LEU:N	2.30	0.44
1:H:57:VAL:HG12	1:H:58:SER:N	2.33	0.44
1:H:190:SER:CB	1:H:191:PRO:HD2	2.48	0.44
3:M:32:GLN:HE22	3:M:107:ASP:H	1.66	0.44
1:H:254:VAL:CG1	1:H:263:LEU:HB3	2.48	0.44
1:E:112:LEU:HD12	1:E:113:ASN:H	1.82	0.44
1:K:99:GLY:N	1:K:103:THR:O	2.42	0.44
3:M:415:VAL:HG13	3:M:418:VAL:HG23	1.99	0.44
2:B:37:VAL:HB	2:B:66:TYR:CE1	2.52	0.44
1:E:99:GLY:O	1:E:100:PRO:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:415:VAL:O	3:J:415:VAL:HG12	2.16	0.44
3:M:151:ALA:HB2	3:M:250:LEU:HD22	1.99	0.44
3:D:112:LEU:O	3:D:113:PRO:C	2.56	0.44
3:G:32:GLN:HE22	3:G:107:ASP:H	1.65	0.44
3:J:112:LEU:O	3:J:113:PRO:C	2.56	0.44
3:D:551:PHE:O	3:D:554:PHE:HB3	2.18	0.44
3:G:34:CYS:HB3	3:G:39:HIS:NE2	2.33	0.44
1:H:241:THR:O	1:H:242:VAL:HG23	2.18	0.44
3:J:349:LEU:HD22	3:J:377:PHE:CG	2.53	0.44
1:K:214:ARG:HB2	1:K:250:TYR:CE2	2.52	0.43
1:A:42:ARG:NH1	3:D:498:VAL:O	2.52	0.43
3:D:135:LEU:HD21	3:D:162:LYS:HB2	1.99	0.43
3:G:551:PHE:O	3:G:554:PHE:HB3	2.18	0.43
3:M:347:LEU:CB	3:M:482:VAL:HG21	2.48	0.43
1:E:68:LEU:HD23	1:E:68:LEU:HA	1.81	0.43
1:E:106:PRO:HG3	1:E:122:LEU:HD22	2.00	0.43
2:F:7:ILE:HD13	2:F:82:VAL:CG2	2.49	0.43
1:K:197:THR:HG21	2:L:99:MET:HG2	2.00	0.43
3:M:472:ARG:NH2	3:M:492:GLU:O	2.52	0.43
3:M:551:PHE:O	3:M:554:PHE:HB3	2.19	0.43
1:A:26:VAL:HG21	1:A:68:LEU:HD13	1.99	0.43
1:H:99:GLY:N	1:H:103:THR:O	2.42	0.43
1:H:203:PHE:CE2	1:H:208:LEU:HD13	2.53	0.43
1:K:83:GLY:O	1:K:84:GLY:O	2.37	0.43
1:A:94:LEU:HD12	1:A:94:LEU:N	2.33	0.43
1:A:214:ARG:HB2	1:A:250:TYR:CE2	2.54	0.43
3:D:44:ASN:O	3:D:48:GLU:HG3	2.19	0.43
3:G:112:LEU:O	3:G:113:PRO:C	2.57	0.43
3:M:133:THR:O	3:M:136:LYS:N	2.52	0.43
3:D:133:THR:O	3:D:136:LYS:N	2.52	0.43
3:D:212:LYS:O	3:D:216:VAL:HG23	2.18	0.43
1:H:42:ARG:NH1	3:J:498:VAL:O	2.52	0.43
1:A:44:GLU:CD	3:D:469:VAL:HG22	2.39	0.43
1:A:203:PHE:CE2	1:A:208:LEU:HD13	2.54	0.43
1:H:126:THR:HA	1:H:142:GLN:HE22	1.84	0.43
1:E:59:TRP:CD1	3:G:463:LEU:HD13	2.54	0.42
1:E:83:GLY:O	1:E:84:GLY:O	2.36	0.42
1:H:56:GLN:NE2	1:H:57:VAL:H	2.17	0.42
3:J:397:GLN:O	3:J:398:LEU:HD23	2.19	0.42
1:K:78:ALA:HB1	1:K:137:ILE:HD13	2.01	0.42
2:B:39:LEU:C	2:B:40:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:281:LYS:HB3	3:M:282:PRO:HD2	2.01	0.42
3:D:526:GLN:O	3:D:530:VAL:HG23	2.19	0.42
3:G:97:GLU:HA	3:G:100:GLU:HG3	2.01	0.42
3:G:415:VAL:O	3:G:415:VAL:CG1	2.68	0.42
3:J:572:GLY:O	3:J:576:VAL:HG23	2.19	0.42
3:D:172:ALA:HB2	3:J:293:VAL:O	2.18	0.42
3:D:281:LYS:HB3	3:D:282:PRO:HD2	2.00	0.42
1:E:122:LEU:HD12	1:E:122:LEU:H	1.84	0.42
3:J:497:TYR:O	3:J:499:PRO:HD3	2.20	0.42
3:G:231:VAL:O	3:G:235:VAL:HG23	2.20	0.42
3:M:326:PHE:HA	3:M:329:MET:HE2	2.01	0.42
1:E:53:TRP:CZ3	3:G:527:THR:HG22	2.54	0.42
3:G:21:ALA:HB1	3:G:139:LEU:HD21	2.02	0.42
3:G:317:LYS:O	3:G:321:GLU:HG2	2.20	0.42
3:M:214:TRP:CD1	3:M:343:VAL:HG11	2.54	0.42
1:E:167:LEU:HD23	1:E:174:LEU:CD1	2.49	0.42
3:J:551:PHE:O	3:J:554:PHE:HB3	2.20	0.42
1:H:56:GLN:HE21	1:H:57:VAL:H	1.67	0.42
3:M:33:GLN:HE21	3:M:112:LEU:HG	1.83	0.42
3:M:497:TYR:O	3:M:499:PRO:HD3	2.20	0.42
1:E:11:LEU:HD12	1:E:11:LEU:N	2.34	0.42
2:F:24:ASN:HB3	2:F:65:LEU:HD11	2.00	0.42
3:G:216:VAL:CG2	3:G:235:VAL:HG21	2.50	0.42
3:G:472:ARG:CZ	3:G:491:LEU:HD22	2.49	0.42
3:G:525:LYS:O	3:G:548:MET:HE1	2.19	0.42
3:M:133:THR:O	3:M:134:PHE:C	2.58	0.42
1:E:59:TRP:CE3	1:E:62:GLU:HG3	2.55	0.42
3:M:97:GLU:HA	3:M:100:GLU:HG3	2.01	0.42
3:G:430:LEU:HD22	3:G:453:LEU:HD23	2.01	0.41
3:J:34:CYS:HB3	3:J:39:HIS:NE2	2.35	0.41
1:K:11:LEU:CD2	1:K:71:LYS:HG2	2.50	0.41
3:D:89:ASP:O	3:D:92:ALA:HB3	2.19	0.41
3:D:412:THR:OG1	3:D:423:LEU:HD13	2.20	0.41
3:M:575:LEU:HD12	3:M:575:LEU:O	2.21	0.41
3:D:317:LYS:O	3:D:321:GLU:HG2	2.21	0.41
3:J:525:LYS:O	3:J:548:MET:HE1	2.20	0.41
3:M:532:LEU:HD13	3:M:547:VAL:HG11	2.02	0.41
1:A:44:GLU:OE2	3:D:469:VAL:HG22	2.20	0.41
1:A:78:ALA:HB1	1:A:137:ILE:HD13	2.02	0.41
3:G:290:ILE:HD13	3:G:290:ILE:HG21	1.88	0.41
3:G:497:TYR:O	3:G:499:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:TRP:CE3	1:H:62:GLU:HG3	2.54	0.41
3:J:347:LEU:CB	3:J:482:VAL:HG21	2.49	0.41
1:A:44:GLU:HG3	3:D:417:GLN:HE21	1.83	0.41
3:G:194:ALA:HB1	3:G:455:VAL:HG11	2.01	0.41
3:J:133:THR:O	3:J:136:LYS:N	2.53	0.41
1:K:59:TRP:CE3	1:K:62:GLU:HG3	2.54	0.41
3:M:119:GLU:O	3:M:122:VAL:HG13	2.20	0.41
3:D:97:GLU:HA	3:D:100:GLU:HG3	2.02	0.41
3:D:494:ASP:OD1	3:D:496:THR:HB	2.21	0.41
3:D:497:TYR:O	3:D:499:PRO:HD3	2.21	0.41
3:G:388:ILE:HD13	3:G:449:ALA:HB2	2.02	0.41
1:K:126:THR:HA	1:K:142:GLN:HE22	1.85	0.41
3:M:349:LEU:HD22	3:M:377:PHE:CG	2.56	0.41
3:M:415:VAL:O	3:M:415:VAL:HG12	2.19	0.41
2:F:27:VAL:HG21	2:F:37:VAL:HG21	2.01	0.41
3:J:42:LEU:HD22	3:J:73:LYS:HG3	2.01	0.41
3:J:408:LEU:HD11	3:J:530:VAL:CG2	2.51	0.41
3:J:415:VAL:O	3:J:415:VAL:HG13	2.21	0.41
1:K:5:LEU:HD23	1:K:5:LEU:HA	1.92	0.41
3:D:71:GLY:HA3	3:D:98:ARG:NH1	2.36	0.41
3:G:293:VAL:HG22	3:G:294:GLU:N	2.36	0.41
3:J:388:ILE:HD13	3:J:449:ALA:HB2	2.02	0.41
2:B:84:HIS:O	2:B:85:VAL:C	2.59	0.41
1:E:78:ALA:HB1	1:E:137:ILE:CD1	2.51	0.41
1:H:21:THR:HG23	1:H:22:PRO:HD2	2.03	0.41
3:J:112:LEU:HA	3:J:112:LEU:HD12	1.84	0.41
3:M:71:GLY:HA3	3:M:98:ARG:NH1	2.36	0.41
1:A:83:GLY:O	1:A:84:GLY:O	2.38	0.41
3:M:217:ALA:HB3	3:M:343:VAL:HG13	2.03	0.41
3:M:25:ILE:O	3:M:26:ALA:C	2.58	0.40
1:A:44:GLU:OE2	3:D:417:GLN:HG3	2.21	0.40
3:J:343:VAL:O	3:J:344:VAL:C	2.60	0.40
1:A:59:TRP:CE3	1:A:62:GLU:HG3	2.56	0.40
3:D:99:ASN:ND2	3:D:103:LEU:CD1	2.84	0.40
1:E:8:LEU:HD23	1:E:95:GLY:HA3	2.04	0.40
3:G:133:THR:O	3:G:136:LYS:N	2.54	0.40
3:G:518:GLU:O	3:G:519:LYS:C	2.60	0.40
3:J:472:ARG:NH1	3:J:491:LEU:HD22	2.37	0.40
1:A:106:PRO:HG2	1:A:122:LEU:HD13	2.03	0.40
3:D:518:GLU:O	3:D:519:LYS:C	2.59	0.40
3:G:412:THR:OG1	3:G:423:LEU:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:541:LYS:NZ	3:J:545:LYS:CE	2.84	0.40
1:A:126:THR:HA	1:A:142:GLN:HE22	1.86	0.40
3:J:97:GLU:HA	3:J:100:GLU:HG3	2.02	0.40
3:J:541:LYS:HZ3	3:J:545:LYS:HE3	1.83	0.40
2:L:89:GLN:O	2:L:90:PRO:C	2.60	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	262/271 (97%)	238 (91%)	19 (7%)	5 (2%)	8	34
1	E	262/271 (97%)	235 (90%)	22 (8%)	5 (2%)	8	34
1	H	262/271 (97%)	235 (90%)	21 (8%)	6 (2%)	6	29
1	K	262/271 (97%)	235 (90%)	22 (8%)	5 (2%)	8	34
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	F	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	I	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	L	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
3	D	581/585 (99%)	534 (92%)	42 (7%)	5 (1%)	17	53
3	G	581/585 (99%)	539 (93%)	37 (6%)	5 (1%)	17	53
3	J	581/585 (99%)	536 (92%)	40 (7%)	5 (1%)	17	53
3	M	581/585 (99%)	541 (93%)	35 (6%)	5 (1%)	17	53
All	All	3760/3820 (98%)	3456 (92%)	263 (7%)	41 (1%)	14	48

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
1	A	191	PRO
3	D	80	LEU
3	D	129	ASP
3	D	442	GLU
1	E	145	ASP
1	E	191	PRO
3	G	80	LEU
3	G	129	ASP
3	G	442	GLU
1	H	145	ASP
1	H	190	SER
1	H	191	PRO
3	J	80	LEU
3	J	129	ASP
3	J	442	GLU
1	K	145	ASP
1	K	191	PRO
3	M	80	LEU
3	M	129	ASP
3	M	442	GLU
1	A	84	GLY
1	E	84	GLY
1	H	84	GLY
1	K	84	GLY
1	A	100	PRO
3	D	113	PRO
1	E	100	PRO
1	H	100	PRO
1	K	100	PRO
3	M	86	GLU
3	D	86	GLU
3	G	86	GLU
3	J	86	GLU
3	J	113	PRO
3	M	113	PRO
1	A	190	SER
1	E	190	SER
3	G	113	PRO
1	K	190	SER
1	H	228	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	218/224 (97%)	203 (93%)	15 (7%)	15	46
1	E	218/224 (97%)	202 (93%)	16 (7%)	14	43
1	H	218/224 (97%)	202 (93%)	16 (7%)	14	43
1	K	218/224 (97%)	203 (93%)	15 (7%)	15	46
2	B	94/94 (100%)	87 (93%)	7 (7%)	13	42
2	F	94/94 (100%)	84 (89%)	10 (11%)	6	25
2	I	94/94 (100%)	88 (94%)	6 (6%)	17	49
2	L	94/94 (100%)	87 (93%)	7 (7%)	13	42
3	D	510/511 (100%)	478 (94%)	32 (6%)	18	49
3	G	510/511 (100%)	477 (94%)	33 (6%)	17	48
3	J	510/511 (100%)	476 (93%)	34 (7%)	16	47
3	M	510/511 (100%)	478 (94%)	32 (6%)	18	49
All	All	3288/3316 (99%)	3065 (93%)	223 (7%)	16	46

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	27	SER
1	A	36	LEU
1	A	116	GLU
1	A	140	ARG
1	A	177	LYS
1	A	190	SER
1	A	194	SER
1	A	214	ARG
1	A	221	THR
1	A	237	SER
1	A	242	VAL
1	A	244	SER
1	A	255	GLN

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Mol	Chain	Res	Type
1	A	261	GLN
2	B	1	ILE
2	B	33	SER
2	B	45	ARG
2	B	70	PHE
2	B	74	GLU
2	B	83	ASN
2	B	94	LYS
3	D	3	HIS
3	D	6	GLU
3	D	34	CYS
3	D	60	GLU
3	D	63	ASP
3	D	76	THR
3	D	79	THR
3	D	98	ARG
3	D	100	GLU
3	D	139	LEU
3	D	193	SER
3	D	222	ARG
3	D	245	CYS
3	D	253	CYS
3	D	257	ARG
3	D	268	GLN
3	D	283	LEU
3	D	292	GLU
3	D	293	VAL
3	D	334	TYR
3	D	337	ARG
3	D	390	GLN
3	D	396	GLU
3	D	433	VAL
3	D	435	SER
3	D	455	VAL
3	D	469	VAL
3	D	484	ARG
3	D	543	GLN
3	D	564	LYS
3	D	565	GLU
3	D	585	LEU
1	E	5	LEU
1	E	10	HIS

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Mol	Chain	Res	Type
1	E	27	SER
1	E	36	LEU
1	E	44	GLU
1	E	116	GLU
1	E	117	PHE
1	E	140	ARG
1	E	190	SER
1	E	194	SER
1	E	214	ARG
1	E	221	THR
1	E	237	SER
1	E	242	VAL
1	E	244	SER
1	E	261	GLN
2	F	1	ILE
2	F	9	VAL
2	F	33	SER
2	F	44	GLU
2	F	47	GLU
2	F	70	PHE
2	F	74	GLU
2	F	83	ASN
2	F	89	GLN
2	F	94	LYS
3	G	3	HIS
3	G	6	GLU
3	G	7	VAL
3	G	34	CYS
3	G	60	GLU
3	G	63	ASP
3	G	79	THR
3	G	98	ARG
3	G	100	GLU
3	G	139	LEU
3	G	193	SER
3	G	204	GLN
3	G	222	ARG
3	G	245	CYS
3	G	253	CYS
3	G	257	ARG
3	G	268	GLN
3	G	334	TYR

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Mol	Chain	Res	Type
3	G	337	ARG
3	G	390	GLN
3	G	396	GLU
3	G	415	VAL
3	G	417	GLN
3	G	424	VAL
3	G	433	VAL
3	G	435	SER
3	G	469	VAL
3	G	478	THR
3	G	484	ARG
3	G	543	GLN
3	G	564	LYS
3	G	565	GLU
3	G	585	LEU
1	H	5	LEU
1	H	10	HIS
1	H	21	THR
1	H	27	SER
1	H	36	LEU
1	H	44	GLU
1	H	116	GLU
1	H	117	PHE
1	H	140	ARG
1	H	194	SER
1	H	214	ARG
1	H	221	THR
1	H	241	THR
1	H	242	VAL
1	H	244	SER
1	H	261	GLN
2	I	1	ILE
2	I	33	SER
2	I	70	PHE
2	I	74	GLU
2	I	83	ASN
2	I	94	LYS
3	J	3	HIS
3	J	6	GLU
3	J	34	CYS
3	J	60	GLU
3	J	63	ASP

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Mol	Chain	Res	Type
3	J	79	THR
3	J	98	ARG
3	J	100	GLU
3	J	139	LEU
3	J	193	SER
3	J	204	GLN
3	J	222	ARG
3	J	245	CYS
3	J	253	CYS
3	J	257	ARG
3	J	268	GLN
3	J	283	LEU
3	J	285	GLU
3	J	292	GLU
3	J	293	VAL
3	J	334	TYR
3	J	337	ARG
3	J	390	GLN
3	J	396	GLU
3	J	415	VAL
3	J	433	VAL
3	J	435	SER
3	J	469	VAL
3	J	482	VAL
3	J	484	ARG
3	J	543	GLN
3	J	564	LYS
3	J	565	GLU
3	J	585	LEU
1	K	10	HIS
1	K	27	SER
1	K	36	LEU
1	K	116	GLU
1	K	117	PHE
1	K	140	ARG
1	K	177	LYS
1	K	190	SER
1	K	194	SER
1	K	214	ARG
1	K	221	THR
1	K	237	SER
1	K	242	VAL

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Mol	Chain	Res	Type
1	K	244	SER
1	K	261	GLN
2	L	1	ILE
2	L	33	SER
2	L	70	PHE
2	L	74	GLU
2	L	83	ASN
2	L	89	GLN
2	L	94	LYS
3	M	3	HIS
3	M	6	GLU
3	M	60	GLU
3	M	79	THR
3	M	98	ARG
3	M	100	GLU
3	M	112	LEU
3	M	139	LEU
3	M	193	SER
3	M	204	GLN
3	M	222	ARG
3	M	245	CYS
3	M	253	CYS
3	M	257	ARG
3	M	268	GLN
3	M	285	GLU
3	M	293	VAL
3	M	334	TYR
3	M	337	ARG
3	M	390	GLN
3	M	396	GLU
3	M	415	VAL
3	M	417	GLN
3	M	433	VAL
3	M	435	SER
3	M	446	MET
3	M	469	VAL
3	M	482	VAL
3	M	484	ARG
3	M	543	GLN
3	M	564	LYS
3	M	565	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	56	GLN
1	A	215	ASN
1	A	255	GLN
1	A	261	GLN
2	B	83	ASN
3	D	33	GLN
3	D	99	ASN
3	D	146	HIS
3	D	535	HIS
3	D	543	GLN
1	E	4	HIS
1	E	56	GLN
1	E	215	ASN
1	E	261	GLN
2	F	83	ASN
3	G	33	GLN
3	G	94	GLN
3	G	535	HIS
3	G	543	GLN
1	H	33	GLN
1	H	56	GLN
1	H	144	GLN
1	H	215	ASN
1	H	261	GLN
2	I	2	GLN
2	I	83	ASN
3	J	33	GLN
3	J	535	HIS
3	J	543	GLN
1	K	33	GLN
1	K	56	GLN
1	K	261	GLN
2	L	83	ASN
3	M	33	GLN
3	M	170	GLN
3	M	535	HIS
3	M	543	GLN

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)

There are no ligands in this entry.

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	264/271 (97%)	-0.48	0	100	100	12, 27, 64, 98	0
1	E	264/271 (97%)	-0.48	0	100	100	12, 28, 63, 87	0
1	H	264/271 (97%)	-0.35	1 (0%)	92	78	15, 34, 70, 104	0
1	K	264/271 (97%)	-0.43	1 (0%)	92	78	13, 31, 70, 95	0
2	B	99/99 (100%)	-0.49	0	100	100	15, 31, 57, 71	0
2	F	99/99 (100%)	-0.40	0	100	100	16, 38, 70, 92	0
2	I	99/99 (100%)	-0.14	1 (1%)	82	58	18, 51, 83, 98	0
2	L	99/99 (100%)	-0.17	0	100	100	16, 49, 79, 96	0
3	D	583/585 (99%)	-0.45	0	100	100	10, 35, 69, 97	0
3	G	583/585 (99%)	-0.47	2 (0%)	94	83	14, 34, 71, 97	0
3	J	583/585 (99%)	-0.45	1 (0%)	95	87	14, 38, 75, 112	0
3	M	583/585 (99%)	-0.43	2 (0%)	94	83	11, 35, 77, 105	0
All	All	3784/3820 (99%)	-0.43	8 (0%)	95	87	10, 34, 73, 112	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	60	GLU	2.8
3	M	116	VAL	2.7
1	K	102	ASN	2.6
3	M	60	GLU	2.5
2	I	73	THR	2.3
3	G	78	ALA	2.1
1	H	187	ARG	2.1
3	G	562	ASP	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.