Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 02:08 PM EDT

PDB ID	:	5XJO
Title	:	Plant receptor ERL1-TMM in complex with peptide EPF1
Authors	:	Chai, J.; Lin, G.; Zhang, L.; Han, Z.; Shpak, E.D.; Yang, X.
Deposited on	:	2017-05-03
Resolution	:	2.63 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:

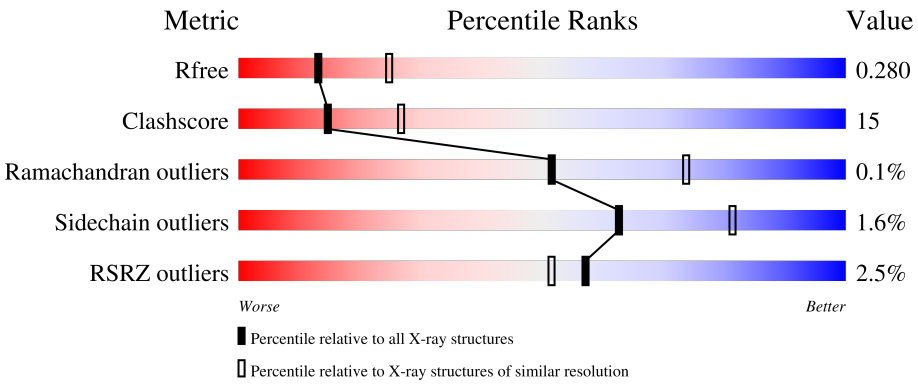
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.63 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	539	69% 27%
1	B	539	2% 70% 26%
2	E	52	8% 60% 19% 19%
2	F	52	4% 62% 19% 19%
3	C	374	3% 66% 32%

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Mol	Chain	Length	Quality of chain
3	D	374	4% 64% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14334 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 LRR receptor-like serine/threonine-protein kinase ERL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	523	3997	2536	680	765	16	0	0	0
1	B	523	3997	2536	680	765	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	ALA	LYS	conflict	UNP C0LGW6
B	546	ALA	LYS	conflict	UNP C0LGW6

- Molecule 2 is a protein called Protein EPIDERMAL PATTERNING FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	42	306	188	54	54	10	0	0	0
2	E	42	306	188	54	54	10	0	0	0

- Molecule 3 is a protein called Protein TOO MANY MOUTHS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	367	2864	1803	521	529	11	0	0	0
3	D	367	2864	1803	521	529	11	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	273	GLN	ILE	conflict	UNP Q9SSD1
C	312	ASN	THR	conflict	UNP Q9SSD1

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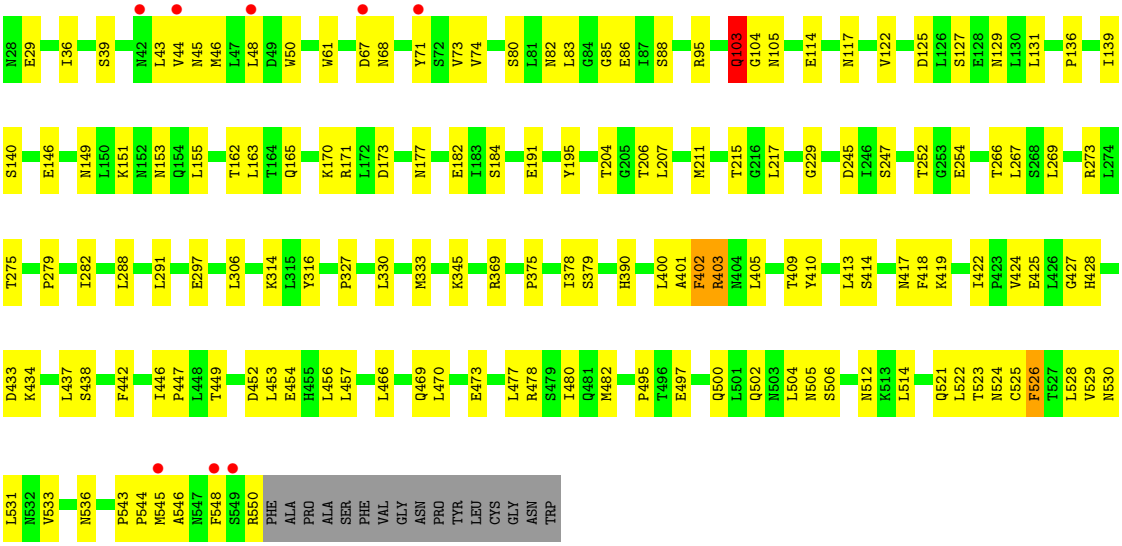
Chain	Residue	Modelled	Actual	Comment	Reference
C	421	ALA	LEU	conflict	UNP Q9SSD1
C	422	ALA	ASP	conflict	UNP Q9SSD1
C	423	ALA	ASP	conflict	UNP Q9SSD1
D	273	GLN	ILE	conflict	UNP Q9SSD1
D	312	ASN	THR	conflict	UNP Q9SSD1
D	421	ALA	LEU	conflict	UNP Q9SSD1
D	422	ALA	ASP	conflict	UNP Q9SSD1
D	423	ALA	ASP	conflict	UNP Q9SSD1

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.

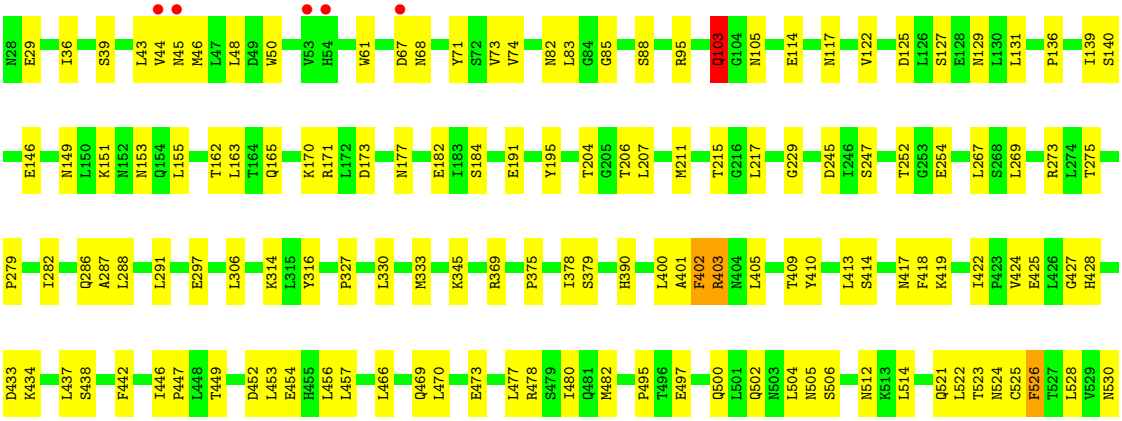
• Molecule 1: LRR receptor-like serine/threonine-protein kinase ERL1

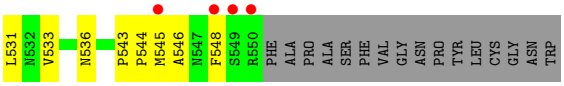
Chain A:



• Molecule 1: LRR receptor-like serine/threonine-protein kinase ERL1

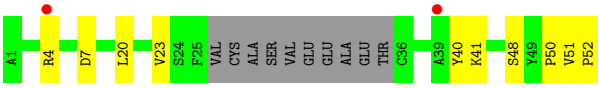
Chain B:





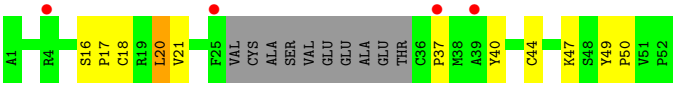
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 1

Chain F:



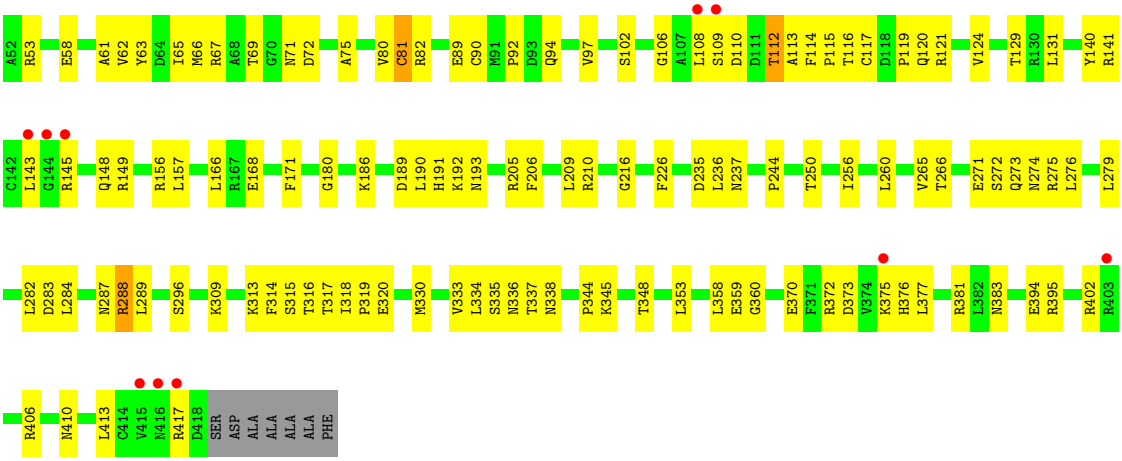
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 1

Chain E:



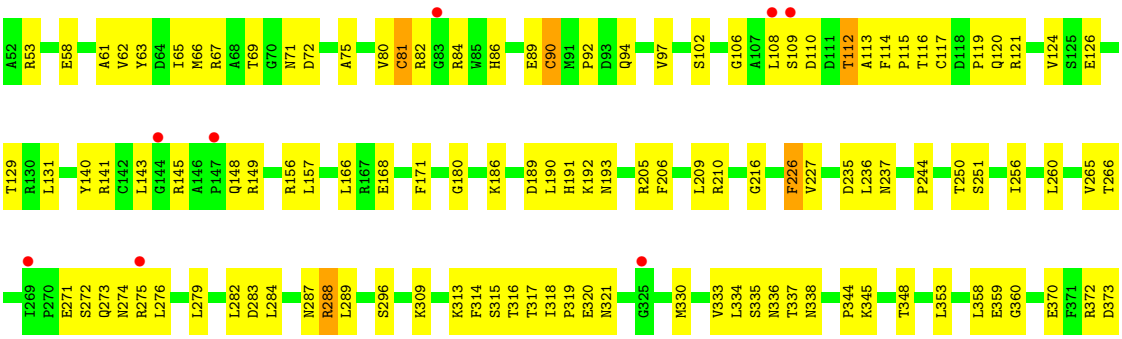
• Molecule 3: Protein TOO MANY MOUTHS

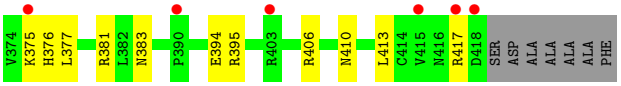
Chain C:



• Molecule 3: Protein TOO MANY MOUTHS

Chain D:




V374
K375
H376
L377
R381
L382
N383
P390
E394
R395
R403
R406
N410
L413
C414
V415
N416
R417
D418
SER
ASP
ALA
ALA
ALA
ALA
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.11Å 66.15Å 143.49Å 97.61° 102.47° 93.68°	Depositor
Resolution (Å)	42.53 – 2.63 46.17 – 2.63	Depositor EDS
% Data completeness (in resolution range)	93.6 (42.53-2.63) 93.7 (46.17-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.252 , 0.310 0.272 , 0.280	Depositor DCC
R_{free} test set	3319 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 12.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14334	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 23.01 % 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 5.0799e-03. 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	0.52	1/4066 (0.0%)	0.67	1/5532 (0.0%)
1	B	0.53	1/4066 (0.0%)	0.67	1/5532 (0.0%)
2	E	0.63	0/313	0.85	1/421 (0.2%)
2	F	0.63	0/313	0.80	0/421
3	C	0.67	1/2920 (0.0%)	0.80	3/3965 (0.1%)
3	D	0.68	2/2920 (0.1%)	0.81	3/3965 (0.1%)
All	All	0.60	5/14598 (0.0%)	0.73	9/19836 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	81	CYS	CB-SG	-7.16	1.70	1.82
3	D	90	CYS	CB-SG	-6.75	1.70	1.82
3	D	81	CYS	CB-SG	-5.72	1.72	1.81
1	B	103	GLN	CD-OE1	-5.21	1.12	1.24
1	A	103	GLN	CD-OE1	-5.20	1.12	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	288	ARG	NE-CZ-NH1	6.67	123.64	120.30
3	C	288	ARG	NE-CZ-NH1	6.59	123.60	120.30
3	D	156	ARG	NE-CZ-NH1	5.73	123.16	120.30
3	C	156	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	163	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	163	LEU	CA-CB-CG	5.46	127.87	115.30
3	C	108	LEU	CA-CB-CG	5.31	127.51	115.30
3	D	108	LEU	CA-CB-CG	5.30	127.49	115.30
2	E	20	LEU	CB-CG-CD2	-5.12	102.29	111.00

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	3997	0	4048	114	4
1	B	3997	0	4048	112	4
2	E	306	0	294	12	0
2	F	306	0	296	11	0
3	C	2864	0	2904	98	4
3	D	2864	0	2904	106	4
All	All	14334	0	14494	440	8

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 15.

All (440) 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:C:53:ARG:NH2	3:C:82:ARG:HH12	1.18	1.36
3:D:53:ARG:NH2	3:D:82:ARG:HH12	1.18	1.34
3:C:53:ARG:HH21	3:C:82:ARG:NH1	1.26	1.29
3:D:53:ARG:HH21	3:D:82:ARG:NH1	1.26	1.29
3:D:81:CYS:SG	3:D:90:CYS:SG	1.26	1.13
3:C:53:ARG:NH2	3:C:82:ARG:NH1	1.85	1.11
3:C:81:CYS:SG	3:C:90:CYS:SG	1.20	1.10
3:D:53:ARG:NH2	3:D:82:ARG:NH1	1.85	1.08
1:B:191:GLU:OE1	1:B:215:THR:OG1	1.73	1.05
3:D:272:SER:HB2	3:D:275:ARG:CZ	1.86	1.05
1:A:191:GLU:OE1	1:A:215:THR:OG1	1.73	1.04
3:C:272:SER:HB2	3:C:275:ARG:CZ	1.86	1.04
1:A:521:GLN:C	1:A:545:MET:HE1	1.79	1.03
1:B:523:THR:HA	1:B:545:MET:HB3	1.47	0.95
1:B:521:GLN:C	1:B:545:MET:HE1	1.85	0.95
1:A:523:THR:HA	1:A:545:MET:HB3	1.47	0.94
3:D:272:SER:HB2	3:D:275:ARG:NH2	1.83	0.94
3:C:272:SER:HB2	3:C:275:ARG:NH2	1.83	0.92
3:D:53:ARG:HH22	3:D:82:ARG:HH12	1.17	0.92
1:A:523:THR:CA	1:A:545:MET:HB3	1.98	0.91
3:C:53:ARG:HH22	3:C:82:ARG:HH12	1.17	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:CYS:CB	3:C:90:CYS:SG	2.60	0.90
3:C:81:CYS:SG	3:C:90:CYS:CB	2.60	0.89
1:B:523:THR:CA	1:B:545:MET:HB3	1.98	0.89
3:D:81:CYS:SG	3:D:90:CYS:CB	2.61	0.89
3:D:81:CYS:HG	3:D:90:CYS:CB	1.86	0.88
1:B:95:ARG:NH2	1:B:117:ASN:HB3	1.91	0.85
1:A:95:ARG:NH2	1:A:117:ASN:HB3	1.91	0.85
3:C:320:GLU:OE2	3:C:345:LYS:N	2.11	0.84
1:B:44:VAL:HG13	1:B:45:ASN:H	1.42	0.84
3:D:320:GLU:OE2	3:D:345:LYS:N	2.11	0.84
1:B:521:GLN:C	1:B:545:MET:CE	2.46	0.84
1:B:155:LEU:H	1:B:177:ASN:HD22	1.26	0.83
1:A:521:GLN:C	1:A:545:MET:CE	2.46	0.83
1:A:44:VAL:HG13	1:A:45:ASN:H	1.42	0.83
3:D:180:GLY:O	3:D:205:ARG:NH1	2.12	0.83
3:C:180:GLY:O	3:C:205:ARG:NH1	2.12	0.82
3:D:348:THR:HG21	3:D:370:GLU:HB3	1.61	0.82
1:A:155:LEU:H	1:A:177:ASN:HD22	1.26	0.81
3:D:81:CYS:CB	3:D:90:CYS:SG	2.68	0.81
3:C:348:THR:HG21	3:C:370:GLU:HB3	1.61	0.81
1:B:433:ASP:HA	1:B:456:LEU:HA	1.64	0.80
1:A:433:ASP:HA	1:A:456:LEU:HA	1.64	0.80
3:C:272:SER:HB2	3:C:275:ARG:NH1	1.97	0.80
3:D:272:SER:HB2	3:D:275:ARG:NH1	1.97	0.78
1:A:43:LEU:HG	1:A:46:MET:HB2	1.66	0.78
1:B:43:LEU:HG	1:B:46:MET:HB2	1.66	0.78
1:A:400:LEU:O	1:A:403:ARG:HG2	1.85	0.77
3:C:81:CYS:HG	3:C:90:CYS:CB	1.92	0.76
1:A:170:LYS:HD3	3:C:109:SER:CB	2.14	0.76
3:C:71:ASN:HD22	3:C:115:PRO:HB3	1.50	0.76
1:B:400:LEU:O	1:B:403:ARG:HG2	1.85	0.76
3:D:109:SER:CB	1:B:170:LYS:HD3	2.16	0.76
3:D:71:ASN:HD22	3:D:115:PRO:HB3	1.50	0.75
1:A:129:ASN:HB2	1:A:153:ASN:HD21	1.51	0.75
1:B:129:ASN:HB2	1:B:153:ASN:HD21	1.51	0.75
1:A:207:LEU:HB3	1:A:211:MET:HE1	1.69	0.75
2:E:44:CYS:O	2:E:47:LYS:HG3	1.86	0.75
3:D:272:SER:CB	3:D:275:ARG:NH2	2.51	0.74
3:C:186:LYS:HB3	3:C:210:ARG:HG2	1.70	0.74
3:C:272:SER:CB	3:C:275:ARG:NH2	2.51	0.73
3:D:186:LYS:HB3	3:D:210:ARG:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LEU:HB3	1:B:211:MET:HE1	1.70	0.73
1:A:524:ASN:H	1:A:545:MET:CE	2.02	0.71
1:B:524:ASN:H	1:B:545:MET:CE	2.03	0.71
3:C:71:ASN:ND2	3:C:115:PRO:HB3	2.06	0.70
1:A:153:ASN:HB2	1:A:177:ASN:HD21	1.57	0.70
3:D:140:TYR:OH	3:D:141:ARG:NH2	2.24	0.70
3:D:316:THR:HG22	3:D:317:THR:H	1.56	0.70
3:D:71:ASN:ND2	3:D:115:PRO:HB3	2.06	0.70
3:C:140:TYR:OH	3:C:141:ARG:NH2	2.24	0.70
1:A:103:GLN:HG3	1:A:127:SER:OG	1.92	0.70
3:C:316:THR:HG22	3:C:317:THR:H	1.56	0.70
1:B:153:ASN:HB2	1:B:177:ASN:HD21	1.57	0.70
1:B:103:GLN:HG3	1:B:127:SER:OG	1.92	0.68
1:B:524:ASN:N	1:B:545:MET:CE	2.57	0.68
1:A:131:LEU:H	1:A:153:ASN:HD22	1.41	0.68
1:B:131:LEU:H	1:B:153:ASN:HD22	1.41	0.68
1:B:330:LEU:HD23	1:B:333:MET:HE1	1.76	0.67
1:A:522:LEU:N	1:A:545:MET:HE1	2.02	0.67
1:A:330:LEU:HD23	1:A:333:MET:HE1	1.77	0.66
1:A:500:GLN:O	1:A:502:GLN:OE1	2.14	0.65
3:C:140:TYR:HH	3:C:141:ARG:NH2	1.94	0.65
1:A:375:PRO:O	1:A:378:ILE:HG22	1.97	0.65
1:A:524:ASN:N	1:A:545:MET:CE	2.56	0.65
3:D:110:ASP:HA	3:D:113:ALA:HB2	1.79	0.64
1:B:425:GLU:OE1	1:B:425:GLU:N	2.23	0.64
1:B:500:GLN:O	1:B:502:GLN:OE1	2.14	0.64
1:B:82:ASN:HA	1:B:105:ASN:HA	1.79	0.64
3:C:110:ASP:HA	3:C:113:ALA:HB2	1.79	0.64
1:A:482:MET:HG2	1:A:506:SER:HB2	1.80	0.64
1:B:375:PRO:O	1:B:378:ILE:HG22	1.97	0.64
1:B:522:LEU:N	1:B:545:MET:HE1	2.04	0.64
1:A:82:ASN:HA	1:A:105:ASN:HA	1.78	0.64
1:A:497:GLU:OE2	1:A:497:GLU:N	2.31	0.64
3:C:235:ASP:OD1	3:C:237:ASN:ND2	2.31	0.64
3:D:120:GLN:O	3:D:145:ARG:HA	1.98	0.64
1:B:43:LEU:HD12	1:B:83:LEU:HD22	1.80	0.64
1:A:521:GLN:O	1:A:545:MET:HE1	1.98	0.63
3:D:140:TYR:HH	3:D:141:ARG:NH2	1.94	0.63
3:C:383:ASN:OD1	3:C:406:ARG:NH2	2.32	0.63
3:D:383:ASN:OD1	3:D:406:ARG:NH2	2.32	0.63
1:B:482:MET:HG2	1:B:506:SER:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLU:N	1:B:497:GLU:OE2	2.31	0.63
3:D:235:ASP:OD1	3:D:237:ASN:ND2	2.31	0.62
3:D:120:GLN:O	3:D:121:ARG:NH1	2.33	0.62
1:B:400:LEU:H	1:B:400:LEU:HD12	1.64	0.62
3:C:120:GLN:O	3:C:145:ARG:HA	1.98	0.62
3:C:120:GLN:O	3:C:121:ARG:NH1	2.33	0.62
1:A:400:LEU:HD12	1:A:400:LEU:H	1.64	0.62
3:C:94:GLN:CD	3:C:94:GLN:H	2.02	0.62
3:C:191:HIS:NE2	3:C:192:LYS:HG3	2.14	0.62
3:D:94:GLN:CD	3:D:94:GLN:H	2.02	0.62
3:D:191:HIS:NE2	3:D:192:LYS:HG3	2.15	0.62
3:D:381:ARG:HD3	3:D:406:ARG:NH2	2.14	0.62
3:C:381:ARG:HD3	3:C:406:ARG:NH2	2.14	0.61
1:A:43:LEU:HD12	1:A:83:LEU:HD22	1.80	0.61
1:A:425:GLU:OE1	1:A:425:GLU:N	2.23	0.61
1:A:345:LYS:HZ1	1:A:369:ARG:HH12	1.49	0.61
1:B:288:LEU:HD13	1:B:291:LEU:HB2	1.83	0.60
3:C:190:LEU:O	3:C:193:ASN:ND2	2.34	0.60
2:F:40:TYR:HB2	2:F:51:VAL:HG11	1.84	0.60
1:B:521:GLN:O	1:B:545:MET:HE1	2.02	0.60
1:B:245:ASP:OD1	1:B:247:SER:OG	2.15	0.60
3:D:272:SER:CB	3:D:275:ARG:HH22	2.15	0.60
3:C:140:TYR:HH	3:C:141:ARG:HH21	1.49	0.59
3:D:190:LEU:O	3:D:193:ASN:ND2	2.35	0.59
1:A:288:LEU:HD13	1:A:291:LEU:HB2	1.83	0.59
1:B:67:ASP:OD1	1:B:74:VAL:HG21	2.03	0.59
1:A:165:GLN:NE2	3:C:283:ASP:OD2	2.34	0.59
1:B:45:ASN:HA	1:B:48:LEU:HG	1.85	0.59
1:A:427:GLY:HA2	1:A:453:LEU:HD11	1.84	0.59
1:A:67:ASP:OD1	1:A:74:VAL:HG21	2.02	0.58
3:C:410:ASN:HB2	3:C:413:LEU:HD12	1.85	0.58
2:E:20:LEU:HD11	2:E:40:TYR:HB3	1.85	0.58
3:C:309:LYS:HB2	3:C:333:VAL:HG12	1.85	0.58
3:D:410:ASN:HB2	3:D:413:LEU:HD12	1.85	0.58
3:D:309:LYS:HB2	3:D:333:VAL:HG12	1.85	0.58
1:B:427:GLY:HA2	1:B:453:LEU:HD11	1.84	0.58
3:C:272:SER:CB	3:C:275:ARG:HH22	2.15	0.58
1:A:45:ASN:HA	1:A:48:LEU:HG	1.85	0.58
2:F:40:TYR:OH	1:B:287:ALA:O	2.17	0.58
3:D:353:LEU:HG	3:D:377:LEU:HD21	1.85	0.57
1:B:413:LEU:HB3	1:B:418:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:LEU:HG	3:C:377:LEU:HD21	1.85	0.57
3:C:372:ARG:HD3	3:C:394:GLU:OE2	2.05	0.57
1:A:245:ASP:OD1	1:A:247:SER:OG	2.15	0.57
1:A:413:LEU:HB3	1:A:418:PHE:CE2	2.39	0.57
3:D:372:ARG:HD3	3:D:394:GLU:OE2	2.05	0.56
1:B:207:LEU:HB3	1:B:211:MET:CE	2.35	0.56
3:D:265:VAL:HG12	3:D:287:ASN:OD1	2.05	0.56
3:C:265:VAL:HG12	3:C:287:ASN:OD1	2.05	0.56
3:D:129:THR:HA	3:D:157:LEU:HD21	1.87	0.56
1:B:531:LEU:HD11	1:B:533:VAL:HG13	1.87	0.56
2:E:47:LYS:HD3	2:E:49:TYR:OH	2.06	0.56
3:D:256:ILE:HA	3:D:279:LEU:HA	1.88	0.56
3:C:129:THR:HA	3:C:157:LEU:HD21	1.87	0.55
3:C:256:ILE:HA	3:C:279:LEU:HA	1.88	0.55
1:B:400:LEU:C	1:B:402:PHE:H	2.10	0.55
1:A:153:ASN:HB2	1:A:177:ASN:ND2	2.22	0.55
1:A:531:LEU:HD11	1:A:533:VAL:HG13	1.87	0.55
3:D:148:GLN:HG2	3:D:149:ARG:N	2.22	0.55
1:B:153:ASN:HB2	1:B:177:ASN:ND2	2.22	0.55
1:A:207:LEU:HB3	1:A:211:MET:CE	2.35	0.55
1:B:345:LYS:HZ1	1:B:369:ARG:HH12	1.54	0.55
3:C:250:THR:OG1	3:C:275:ARG:NH2	2.40	0.55
1:A:446:ILE:HD11	1:A:466:LEU:HD13	1.89	0.54
1:A:505:ASN:HA	1:A:528:LEU:HA	1.89	0.54
3:D:283:ASP:OD2	1:B:165:GLN:NE2	2.38	0.54
1:B:114:GLU:OE1	1:B:114:GLU:N	2.33	0.54
1:A:400:LEU:C	1:A:402:PHE:H	2.10	0.54
3:C:148:GLN:HG2	3:C:149:ARG:N	2.22	0.54
3:C:276:LEU:HD12	3:C:279:LEU:HD22	1.89	0.54
1:B:345:LYS:NZ	1:B:369:ARG:HH12	2.04	0.54
1:B:151:LYS:HE2	1:B:173:ASP:OD2	2.07	0.54
1:A:345:LYS:NZ	1:A:369:ARG:HH12	2.04	0.54
1:B:446:ILE:HD11	1:B:466:LEU:HD13	1.89	0.54
1:B:505:ASN:HA	1:B:528:LEU:HA	1.89	0.54
3:C:273:GLN:NE2	3:C:282:LEU:HD11	2.23	0.54
3:D:315:SER:OG	3:D:338:ASN:OD1	2.15	0.54
3:D:395:ARG:NH2	3:D:417:ARG:HB3	2.23	0.54
3:D:250:THR:OG1	3:D:275:ARG:NH2	2.40	0.54
1:A:151:LYS:HE2	1:A:173:ASP:OD2	2.07	0.54
2:F:23:VAL:HG22	2:F:41:LYS:HE2	1.90	0.54
3:C:315:SER:OG	3:C:338:ASN:OD1	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:272:SER:CB	3:D:275:ARG:NH1	2.71	0.53
3:D:273:GLN:NE2	3:D:282:LEU:HD11	2.23	0.53
3:D:317:THR:O	3:D:319:PRO:HD3	2.08	0.53
2:F:50:PRO:HB3	3:D:112:THR:HA	1.90	0.53
2:E:50:PRO:HB3	3:C:112:THR:HG23	1.89	0.53
3:D:276:LEU:HD12	3:D:279:LEU:HD22	1.89	0.53
3:C:317:THR:O	3:C:319:PRO:HD3	2.08	0.53
1:B:473:GLU:OE2	1:B:473:GLU:N	2.36	0.53
3:C:121:ARG:HA	3:C:145:ARG:HB3	1.91	0.53
1:B:452:ASP:OD1	1:B:452:ASP:O	2.26	0.53
1:A:425:GLU:H	1:A:425:GLU:CD	2.07	0.53
3:C:191:HIS:NE2	3:C:192:LYS:CD	2.71	0.53
3:C:334:LEU:HB2	3:C:358:LEU:HD23	1.91	0.53
3:C:395:ARG:NH2	3:C:417:ARG:HB3	2.23	0.53
3:D:121:ARG:HA	3:D:145:ARG:HB3	1.91	0.53
3:D:191:HIS:NE2	3:D:192:LYS:CD	2.71	0.53
3:C:120:GLN:HG2	3:C:121:ARG:HD2	1.90	0.53
3:C:206:PHE:HB3	3:C:209:LEU:HB2	1.90	0.53
3:D:191:HIS:CE1	3:D:192:LYS:HG3	2.44	0.53
3:D:206:PHE:HB3	3:D:209:LEU:HB2	1.90	0.53
3:D:334:LEU:HB2	3:D:358:LEU:HD23	1.91	0.53
1:A:114:GLU:OE1	1:A:114:GLU:N	2.33	0.53
1:A:514:LEU:H	1:A:536:ASN:HD22	1.57	0.52
3:C:67:ARG:HD3	3:C:72:ASP:OD2	2.10	0.52
3:D:67:ARG:HD3	3:D:72:ASP:OD2	2.10	0.52
3:D:353:LEU:HG	3:D:377:LEU:CD2	2.40	0.52
1:A:452:ASP:O	1:A:452:ASP:OD1	2.26	0.52
3:C:191:HIS:CE1	3:C:192:LYS:HG3	2.44	0.52
3:D:120:GLN:HG2	3:D:121:ARG:HD2	1.90	0.52
3:C:272:SER:CB	3:C:275:ARG:NH1	2.71	0.52
1:A:469:GLN:HG2	1:A:470:LEU:N	2.25	0.51
1:B:469:GLN:HG2	1:B:470:LEU:N	2.25	0.51
3:C:353:LEU:HG	3:C:377:LEU:CD2	2.40	0.51
1:B:514:LEU:H	1:B:536:ASN:HD22	1.57	0.51
1:A:252:THR:HG21	1:A:273:ARG:NH1	2.25	0.51
3:C:271:GLU:H	3:C:271:GLU:CD	2.13	0.51
3:D:106:GLY:O	3:D:114:PHE:HB2	2.11	0.51
1:B:252:THR:HG21	1:B:273:ARG:NH1	2.25	0.51
1:B:506:SER:HA	1:B:530:ASN:O	2.11	0.51
3:C:191:HIS:CE1	3:C:192:LYS:HE3	2.45	0.51
1:A:506:SER:HA	1:A:530:ASN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:HG13	1:A:146:GLU:HG3	1.92	0.50
3:D:63:TYR:CD1	3:D:75:ALA:HA	2.46	0.50
3:C:63:TYR:CD1	3:C:75:ALA:HA	2.46	0.50
3:D:191:HIS:CE1	3:D:192:LYS:HE3	2.45	0.50
1:B:400:LEU:C	1:B:402:PHE:N	2.64	0.50
1:A:400:LEU:O	1:A:402:PHE:N	2.45	0.50
1:B:400:LEU:O	1:B:402:PHE:N	2.45	0.50
2:F:7:ASP:O	2:F:52:PRO:HG2	2.11	0.50
3:C:106:GLY:O	3:C:114:PHE:HB2	2.11	0.50
3:D:271:GLU:H	3:D:271:GLU:CD	2.13	0.50
3:D:318:ILE:O	3:D:344:PRO:HG3	2.11	0.50
1:B:122:VAL:HG13	1:B:146:GLU:HG3	1.92	0.50
3:C:318:ILE:O	3:C:344:PRO:HG3	2.11	0.50
1:B:36:ILE:HA	1:B:88:SER:HB3	1.93	0.50
1:B:433:ASP:HB2	1:B:457:LEU:HG	1.94	0.49
1:A:473:GLU:OE2	1:A:473:GLU:N	2.36	0.49
3:C:276:LEU:CD1	3:C:279:LEU:HD22	2.43	0.49
3:C:186:LYS:HA	3:C:209:LEU:HA	1.94	0.49
3:C:189:ASP:OD2	3:C:191:HIS:HB3	2.12	0.49
3:D:189:ASP:OD2	3:D:191:HIS:HB3	2.12	0.49
1:B:67:ASP:OD2	1:B:74:VAL:HG11	2.13	0.49
1:A:67:ASP:OD2	1:A:74:VAL:HG11	2.13	0.49
1:A:400:LEU:C	1:A:402:PHE:N	2.64	0.49
3:C:148:GLN:HG2	3:C:149:ARG:O	2.13	0.49
1:A:182:GLU:HA	1:A:204:THR:O	2.13	0.48
3:C:119:PRO:HA	3:C:143:LEU:O	2.13	0.48
3:D:276:LEU:CD1	3:D:279:LEU:HD22	2.43	0.48
1:A:36:ILE:HA	1:A:88:SER:HB3	1.93	0.48
1:A:433:ASP:HB2	1:A:457:LEU:HG	1.94	0.48
2:E:20:LEU:HD11	2:E:40:TYR:HD1	1.77	0.48
3:D:148:GLN:HG2	3:D:149:ARG:O	2.13	0.48
1:B:424:VAL:N	1:B:425:GLU:OE1	2.47	0.48
1:A:413:LEU:HB3	1:A:418:PHE:HE2	1.78	0.48
3:D:315:SER:HA	3:D:338:ASN:O	2.13	0.48
1:B:182:GLU:HA	1:B:204:THR:O	2.13	0.48
3:D:186:LYS:HA	3:D:209:LEU:HA	1.94	0.48
1:A:306:LEU:O	1:A:333:MET:HE2	2.13	0.48
3:D:119:PRO:HA	3:D:143:LEU:O	2.13	0.48
3:D:166:LEU:HB3	3:D:171:PHE:HE2	1.79	0.48
1:A:543:PRO:HA	1:A:544:PRO:HD3	1.72	0.48
3:C:315:SER:HA	3:C:338:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:O	1:A:85:GLY:HA3	2.14	0.48
1:A:424:VAL:N	1:A:425:GLU:OE1	2.47	0.48
1:B:306:LEU:O	1:B:333:MET:HE2	2.14	0.48
1:B:502:GLN:HG3	1:B:526:PHE:HE1	1.79	0.48
3:C:191:HIS:NE2	3:C:192:LYS:CG	2.77	0.48
3:D:314:PHE:HB3	3:D:337:THR:O	2.14	0.48
1:A:502:GLN:HG3	1:A:526:PHE:HE1	1.79	0.47
3:C:166:LEU:HB3	3:C:171:PHE:HE2	1.79	0.47
3:D:191:HIS:NE2	3:D:192:LYS:HD2	2.29	0.47
1:A:275:THR:HG22	1:A:297:GLU:HB2	1.96	0.47
2:E:16:SER:O	2:E:18:CYS:N	2.45	0.47
1:B:413:LEU:HB3	1:B:418:PHE:HE2	1.78	0.47
1:B:275:THR:HG22	1:B:297:GLU:HB2	1.96	0.47
2:E:17:PRO:HD2	2:E:44:CYS:SG	2.55	0.47
3:C:191:HIS:NE2	3:C:192:LYS:HD2	2.29	0.47
3:D:191:HIS:NE2	3:D:192:LYS:CG	2.77	0.47
1:B:279:PRO:HD2	1:B:282:ILE:HD12	1.96	0.47
3:C:314:PHE:HB3	3:C:337:THR:O	2.14	0.47
1:B:171:ARG:HG3	1:B:195:TYR:HB3	1.97	0.47
3:D:67:ARG:CD	3:D:72:ASP:OD2	2.63	0.47
1:B:44:VAL:HG13	1:B:45:ASN:N	2.21	0.47
1:A:279:PRO:HD2	1:A:282:ILE:HD12	1.96	0.47
3:C:244:PRO:HA	3:C:266:THR:O	2.14	0.47
1:A:44:VAL:CG1	1:A:45:ASN:H	2.22	0.47
3:C:67:ARG:CD	3:C:72:ASP:OD2	2.63	0.47
1:B:39:SER:O	1:B:85:GLY:HA3	2.14	0.47
1:A:171:ARG:HG3	1:A:195:TYR:HB3	1.97	0.46
3:D:244:PRO:HA	3:D:266:THR:O	2.14	0.46
1:A:379:SER:HA	1:A:405:LEU:HD21	1.97	0.46
2:E:20:LEU:HD12	2:E:21:VAL:N	2.31	0.46
1:A:446:ILE:CD1	1:A:466:LEU:HD13	2.46	0.46
1:B:425:GLU:H	1:B:425:GLU:CD	2.07	0.46
1:B:314:LYS:HE2	1:B:316:TYR:OH	2.16	0.46
2:F:50:PRO:HB3	3:D:112:THR:HG23	1.98	0.46
3:C:63:TYR:CE1	3:C:75:ALA:HA	2.51	0.46
3:D:120:GLN:O	3:D:121:ARG:HD2	2.15	0.46
3:C:120:GLN:O	3:C:121:ARG:HD2	2.15	0.46
3:C:236:LEU:HD12	3:C:260:LEU:CD2	2.46	0.46
3:D:236:LEU:HD12	3:D:260:LEU:CD2	2.45	0.46
1:A:314:LYS:HE2	1:A:316:TYR:OH	2.16	0.46
3:D:63:TYR:CE1	3:D:75:ALA:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ILE:CD1	1:B:466:LEU:HD13	2.46	0.46
3:C:92:PRO:HA	3:C:97:VAL:O	2.16	0.45
3:D:92:PRO:HA	3:D:97:VAL:O	2.16	0.45
1:B:546:ALA:HB1	1:B:548:PHE:CE2	2.51	0.45
1:B:379:SER:HA	1:B:405:LEU:HD21	1.97	0.45
1:A:345:LYS:NZ	1:A:369:ARG:NH1	2.65	0.45
2:E:44:CYS:O	2:E:47:LYS:CG	2.62	0.45
1:A:546:ALA:HB1	1:A:548:PHE:CE2	2.51	0.45
3:C:359:GLU:HB2	3:C:383:ASN:O	2.17	0.45
1:A:330:LEU:HD23	1:A:333:MET:CE	2.45	0.45
1:A:470:LEU:HD23	1:A:495:PRO:HD3	1.98	0.45
3:D:66:MET:O	3:D:69:THR:HG22	2.17	0.45
1:B:345:LYS:NZ	1:B:369:ARG:NH1	2.65	0.45
1:B:267:LEU:HD11	1:B:269:LEU:HD21	1.99	0.44
1:A:521:GLN:O	1:A:545:MET:CE	2.63	0.44
1:A:378:ILE:O	1:A:378:ILE:HG13	2.17	0.44
1:B:44:VAL:CG1	1:B:45:ASN:H	2.22	0.44
1:A:500:GLN:O	1:A:502:GLN:CD	2.56	0.44
1:B:500:GLN:O	1:B:502:GLN:CD	2.56	0.44
1:A:50:TRP:CD1	1:A:61:TRP:HB3	2.53	0.44
3:C:66:MET:O	3:C:69:THR:HG22	2.17	0.44
3:D:359:GLU:HB2	3:D:383:ASN:O	2.17	0.44
1:B:140:SER:HB3	1:B:162:THR:HB	2.00	0.44
1:A:400:LEU:HD23	1:A:425:GLU:OE2	2.17	0.44
1:B:470:LEU:HD23	1:B:495:PRO:HD3	1.98	0.44
2:F:20:LEU:HD11	2:F:40:TYR:HB3	1.99	0.43
1:B:330:LEU:HD23	1:B:333:MET:CE	2.45	0.43
1:B:400:LEU:HD23	1:B:425:GLU:OE2	2.17	0.43
1:A:390:HIS:HA	1:A:414:SER:O	2.18	0.43
1:A:437:LEU:HB3	1:A:442:PHE:CE2	2.52	0.43
1:B:50:TRP:CD1	1:B:61:TRP:HB3	2.53	0.43
1:B:437:LEU:HB3	1:B:442:PHE:CE2	2.52	0.43
1:A:129:ASN:HB2	1:A:153:ASN:ND2	2.27	0.43
2:E:20:LEU:HD11	2:E:40:TYR:CD1	2.53	0.43
3:C:89:GLU:HB2	3:C:102:SER:HB3	2.01	0.43
3:D:124:VAL:H	3:D:148:GLN:HE22	1.67	0.43
3:D:274:ASN:HD21	3:D:296:SER:HB3	1.83	0.43
3:C:274:ASN:HD21	3:C:296:SER:HB3	1.83	0.43
1:A:267:LEU:HD11	1:A:269:LEU:HD21	1.99	0.43
3:D:266:THR:HG22	3:D:288:ARG:HB2	2.00	0.43
1:A:86:GLU:OE2	3:C:402:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HG2	1:A:275:THR:O	2.19	0.43
3:C:336:ASN:HA	3:C:360:GLY:O	2.19	0.43
3:D:89:GLU:HB2	3:D:102:SER:HB3	2.00	0.43
1:B:254:GLU:HG2	1:B:275:THR:O	2.19	0.43
1:A:417:ASN:OD1	1:A:419:LYS:NZ	2.52	0.43
3:D:66:MET:HA	3:D:69:THR:HG22	2.01	0.43
1:B:417:ASN:O	1:B:419:LYS:NZ	2.51	0.43
1:B:425:GLU:HA	1:B:428:HIS:ND1	2.34	0.43
3:C:266:THR:HG22	3:C:288:ARG:HB2	2.00	0.43
1:A:125:ASP:OD1	1:A:149:ASN:ND2	2.52	0.43
1:B:521:GLN:O	1:B:545:MET:CE	2.63	0.43
1:A:417:ASN:O	1:A:419:LYS:NZ	2.51	0.42
1:A:504:LEU:HD11	1:A:506:SER:O	2.20	0.42
3:C:66:MET:HA	3:C:69:THR:HG22	2.01	0.42
1:B:125:ASP:OD1	1:B:149:ASN:ND2	2.52	0.42
1:B:378:ILE:HG13	1:B:378:ILE:O	2.17	0.42
1:B:546:ALA:HB1	1:B:548:PHE:CD2	2.54	0.42
3:C:124:VAL:H	3:C:148:GLN:HE22	1.66	0.42
1:B:390:HIS:HA	1:B:414:SER:O	2.19	0.42
3:D:227:VAL:HG13	3:D:251:SER:HB2	2.02	0.42
1:B:129:ASN:HB2	1:B:153:ASN:ND2	2.27	0.42
1:A:410:TYR:HD1	1:A:434:LYS:HB2	1.85	0.42
1:A:477:LEU:O	1:A:480:ILE:HG22	2.20	0.42
3:D:191:HIS:CD2	3:D:192:LYS:HG3	2.54	0.42
3:D:192:LYS:HA	3:D:216:GLY:O	2.19	0.42
1:B:410:TYR:HD1	1:B:434:LYS:HB2	1.85	0.42
1:B:504:LEU:HD11	1:B:506:SER:O	2.20	0.42
1:A:140:SER:HB3	1:A:162:THR:HB	2.00	0.42
1:A:378:ILE:CG2	1:A:402:PHE:HE1	2.33	0.42
3:D:126:GLU:O	3:D:129:THR:OG1	2.30	0.42
3:D:336:ASN:HA	3:D:360:GLY:O	2.19	0.42
1:B:477:LEU:O	1:B:480:ILE:HG22	2.20	0.42
1:A:425:GLU:HA	1:A:428:HIS:ND1	2.34	0.42
3:C:191:HIS:CD2	3:C:192:LYS:HG3	2.54	0.42
1:A:266:THR:HG21	2:E:37:PRO:HB3	2.00	0.42
1:B:427:GLY:HA3	1:B:449:THR:HB	2.02	0.42
1:A:427:GLY:HA3	1:A:449:THR:HB	2.02	0.42
1:B:417:ASN:OD1	1:B:419:LYS:NZ	2.52	0.42
1:A:546:ALA:HB1	1:A:548:PHE:CD2	2.54	0.42
2:F:51:VAL:O	3:D:86:HIS:HB2	2.20	0.42
1:B:378:ILE:CG2	1:B:402:PHE:HE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:CYS:HB3	1:B:528:LEU:HB2	2.02	0.42
3:C:61:ALA:O	3:C:65:ILE:HD12	2.20	0.41
3:C:141:ARG:NH1	3:C:168:GLU:OE2	2.53	0.41
3:C:192:LYS:HA	3:C:216:GLY:O	2.19	0.41
3:D:58:GLU:HG2	3:D:131:LEU:HD23	2.02	0.41
1:A:136:PRO:HD2	1:A:139:ILE:HG13	2.02	0.41
3:C:335:SER:O	3:C:337:THR:HG23	2.20	0.41
3:D:61:ALA:O	3:D:65:ILE:HD12	2.20	0.41
1:A:252:THR:HG22	1:A:273:ARG:HB2	2.02	0.41
1:A:327:PRO:O	1:A:330:LEU:HD12	2.20	0.41
2:F:4:ARG:HA	1:B:286:GLN:HB2	2.03	0.41
2:F:41:LYS:HD2	2:F:48:SER:HB2	2.01	0.41
3:D:141:ARG:NH1	3:D:168:GLU:OE2	2.53	0.41
1:B:422:ILE:HG22	1:B:447:PRO:HG2	2.03	0.41
1:A:414:SER:HA	1:A:438:SER:O	2.20	0.41
1:A:525:CYS:HB3	1:A:528:LEU:HB2	2.02	0.41
2:F:52:PRO:HA	3:D:86:HIS:N	2.36	0.41
2:E:20:LEU:HD12	2:E:21:VAL:H	1.85	0.41
1:A:422:ILE:HG22	1:A:447:PRO:HG2	2.03	0.41
1:B:29:GLU:OE1	1:B:73:VAL:HG23	2.21	0.41
1:B:136:PRO:HD2	1:B:139:ILE:HG13	2.02	0.41
3:D:226:PHE:C	3:D:226:PHE:CD1	2.93	0.41
1:A:512:ASN:HB2	1:A:536:ASN:HD21	1.86	0.41
3:C:116:THR:HG22	3:C:117:CYS:N	2.36	0.41
1:B:95:ARG:HH22	1:B:117:ASN:HB3	1.80	0.41
1:A:29:GLU:OE1	1:A:73:VAL:HG23	2.21	0.41
3:D:62:VAL:HG11	3:D:80:VAL:HG11	2.02	0.41
3:D:226:PHE:C	3:D:226:PHE:HD1	2.24	0.41
3:D:321:ASN:N	3:D:321:ASN:HD22	2.19	0.41
1:B:206:THR:HG22	1:B:229:GLY:HA3	2.03	0.41
1:B:252:THR:HG22	1:B:273:ARG:HB2	2.02	0.41
1:B:512:ASN:HB2	1:B:536:ASN:HD21	1.86	0.41
1:B:543:PRO:HA	1:B:544:PRO:HD3	1.72	0.41
3:D:284:LEU:HB3	3:D:289:LEU:HD11	2.03	0.41
1:B:327:PRO:O	1:B:330:LEU:HD12	2.20	0.41
1:A:44:VAL:HG13	1:A:45:ASN:N	2.21	0.40
3:C:62:VAL:HG11	3:C:80:VAL:HG11	2.02	0.40
3:D:116:THR:HG22	3:D:117:CYS:N	2.36	0.40
3:D:335:SER:O	3:D:337:THR:HG23	2.20	0.40
3:C:330:MET:HA	3:C:353:LEU:HA	2.03	0.40
1:A:524:ASN:H	1:A:545:MET:HE3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:HG2	3:C:131:LEU:HD23	2.02	0.40
3:C:284:LEU:HB3	3:C:289:LEU:HD11	2.03	0.40
3:D:273:GLN:HE21	3:D:282:LEU:HD11	1.84	0.40
3:D:330:MET:HA	3:D:353:LEU:HA	2.04	0.40
1:B:414:SER:HA	1:B:438:SER:O	2.20	0.40
1:A:206:THR:HG22	1:A:229:GLY:HA3	2.03	0.40
1:A:529:VAL:HG22	1:A:550:ARG:HB2	2.04	0.40
1:A:80:SER:HA	1:A:104:GLY:O	2.22	0.40
3:D:84:ARG:HH21	3:D:89:GLU:HA	1.87	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:375:LYS:NZ	1:B:454:GLU:OE1[1_655]	1.90	0.30
1:A:478:ARG:NH2	3:C:373:ASP:OD2[1_565]	1.94	0.26
3:D:373:ASP:OD2	1:B:478:ARG:NH2[1_655]	1.94	0.26
1:A:454:GLU:OE1	3:C:375:LYS:NZ[1_565]	1.98	0.22
3:D:375:LYS:NZ	1:B:454:GLU:CD[1_655]	2.11	0.09
3:D:375:LYS:NZ	1:B:454:GLU:OE2[1_655]	2.11	0.09
1:A:454:GLU:OE2	3:C:375:LYS:NZ[1_565]	2.15	0.05
1:A:454:GLU:CD	3:C:375:LYS:NZ[1_565]	2.17	0.03

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	521/539 (97%)	464 (89%)	56 (11%)	1 (0%)	47 69
1	B	521/539 (97%)	464 (89%)	56 (11%)	1 (0%)	47 69
2	E	38/52 (73%)	35 (92%)	3 (8%)	0	100 100
2	F	38/52 (73%)	36 (95%)	2 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	365/374 (98%)	331 (91%)	34 (9%)	0	100	100
3	D	365/374 (98%)	331 (91%)	34 (9%)	0	100	100
All	All	1848/1930 (96%)	1661 (90%)	185 (10%)	2 (0%)	51	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ALA
1	B	401	ALA

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	459/471 (98%)	450 (98%)	9 (2%)	55	77
1	B	459/471 (98%)	450 (98%)	9 (2%)	55	77
2	E	37/45 (82%)	37 (100%)	0	100	100
2	F	37/45 (82%)	37 (100%)	0	100	100
3	C	324/328 (99%)	320 (99%)	4 (1%)	71	86
3	D	324/328 (99%)	320 (99%)	4 (1%)	71	86
All	All	1640/1688 (97%)	1614 (98%)	26 (2%)	62	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	71	TYR
1	A	103	GLN
1	A	184	SER
1	A	217	LEU
1	A	402	PHE
1	A	403	ARG
1	A	409	THR

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Mol	Chain	Res	Type
1	A	526	PHE
3	C	112	THR
3	C	226	PHE
3	C	313	LYS
3	C	376	HIS
3	D	112	THR
3	D	226	PHE
3	D	313	LYS
3	D	376	HIS
1	B	68	ASN
1	B	71	TYR
1	B	103	GLN
1	B	184	SER
1	B	217	LEU
1	B	402	PHE
1	B	403	ARG
1	B	409	THR
1	B	526	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	177	ASN
1	A	286	GLN
1	A	481	GLN
1	A	536	ASN
3	C	71	ASN
3	C	148	GLN
3	C	169	ASN
3	C	321	ASN
3	C	351	ASN
3	D	71	ASN
3	D	148	GLN
3	D	169	ASN
3	D	321	ASN
3	D	351	ASN
1	B	153	ASN
1	B	177	ASN
1	B	286	GLN
1	B	481	GLN
1	B	536	ASN

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	523/539 (97%)	-0.04	8 (1%)	73	70	27, 38, 62, 84	0
1	B	523/539 (97%)	0.10	9 (1%)	70	66	27, 38, 62, 84	0
2	E	42/52 (80%)	0.51	4 (9%)	8	5	35, 50, 57, 59	0
2	F	42/52 (80%)	0.32	2 (4%)	30	24	38, 51, 58, 64	0
3	C	367/374 (98%)	0.13	10 (2%)	54	49	25, 40, 60, 77	0
3	D	367/374 (98%)	0.21	14 (3%)	40	34	25, 40, 60, 77	0
All	All	1864/1930 (96%)	0.10	47 (2%)	57	51	25, 39, 61, 84	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	SER	9.1
3	C	144	GLY	6.7
3	C	145	ARG	5.7
3	C	415	VAL	4.6
3	C	108	LEU	4.4
3	C	143	LEU	4.3
3	C	417	ARG	4.1
3	C	109	SER	4.0
1	A	44	VAL	3.9
3	D	108	LEU	3.9
1	A	549	SER	3.8
1	A	67	ASP	3.7
3	C	416	ASN	3.7
1	B	53	VAL	3.7
1	A	48	LEU	3.6
2	E	25	PHE	3.6
3	D	417	ARG	3.6
3	D	415	VAL	3.5
1	B	67	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	545	MET	3.4
3	D	403	ARG	3.3
3	D	147	PRO	3.2
2	E	4	ARG	3.2
2	E	39	ALA	3.2
1	B	44	VAL	3.1
3	D	109	SER	3.1
1	A	71	TYR	2.9
1	B	550	ARG	2.9
1	A	545	MET	2.8
3	D	144	GLY	2.8
3	D	418	ASP	2.8
1	A	548	PHE	2.8
2	F	4	ARG	2.6
3	C	375	LYS	2.5
3	C	403	ARG	2.5
3	D	269	ILE	2.5
1	B	45	ASN	2.4
3	D	375	LYS	2.3
1	B	54	HIS	2.3
1	A	42	ASN	2.2
2	E	37	PRO	2.2
1	B	548	PHE	2.2
3	D	390	PRO	2.2
2	F	39	ALA	2.2
3	D	83	GLY	2.0
3	D	325	GLY	2.0
3	D	275	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.