



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:10 PM UTC

PDB ID : 2JJD / pdb_00002jjd
Title : Protein Tyrosine Phosphatase, Receptor Type, E isoform
Authors : Elkins, J.M.; Ugochukwu, E.; Alfano, I.; Barr, A.J.; Bunkoczi, G.; King, O.N.F.; Filippakopoulos, P.; Savitsky, P.; Salah, E.; Pike, A.; Johansson, C.; Das, S.; Burgess-Brown, N.A.; Gileadi, O.; von Delft, F.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.M.; Knapp, S.
Deposited on : 2008-03-31
Resolution : 3.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

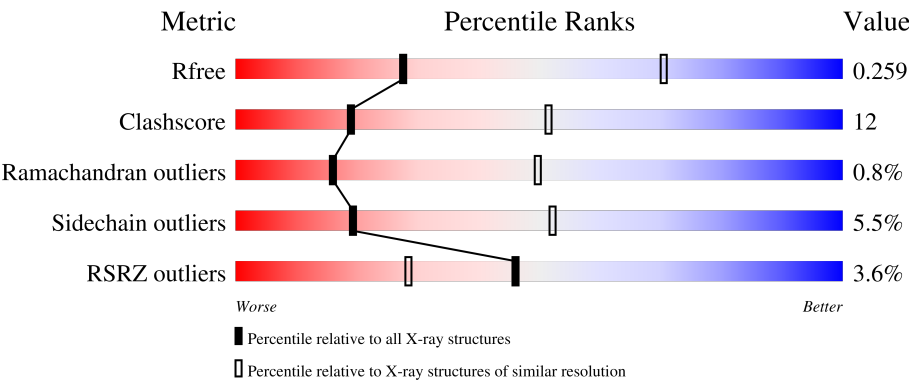
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	599	
1	B	599	
1	C	599	
1	D	599	
1	E	599	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	599	3% 71% 18% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23750 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 RECEPTOR-TYPE TYROSINE-PROTEIN PHOSPHATASE EPSILON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			3973	2574	689	689	21			
1	B	541	Total	C	N	O	S	0	0	0
			3972	2581	692	677	22			
1	C	541	Total	C	N	O	S	0	0	0
			3970	2582	690	676	22			
1	D	539	Total	C	N	O	S	0	0	0
			3936	2554	690	671	21			
1	E	541	Total	C	N	O	S	0	0	0
			3950	2569	688	672	21			
1	F	542	Total	C	N	O	S	0	0	0
			3937	2560	692	664	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	581	GLY	GLU	cloning artifact	UNP P23469
B	581	GLY	GLU	cloning artifact	UNP P23469
C	581	GLY	GLU	cloning artifact	UNP P23469
D	581	GLY	GLU	cloning artifact	UNP P23469
E	581	GLY	GLU	cloning artifact	UNP P23469
F	581	GLY	GLU	cloning artifact	UNP P23469

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	3	Total	Cl	0	0
			3	3		
2	C	1	Total	Cl	0	0
			1	1		

Continued on next page...

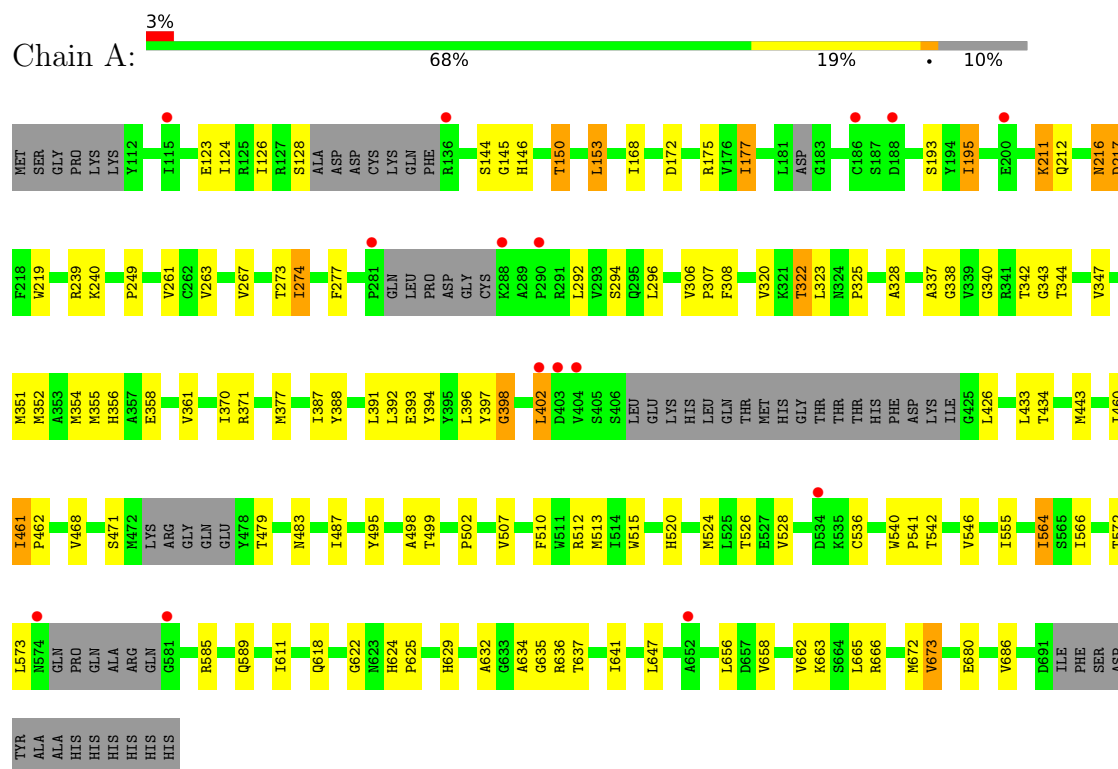
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Cl 2	0	0
2	E	2	Total 2	Cl 2	0	0
2	F	2	Total 2	Cl 2	0	0

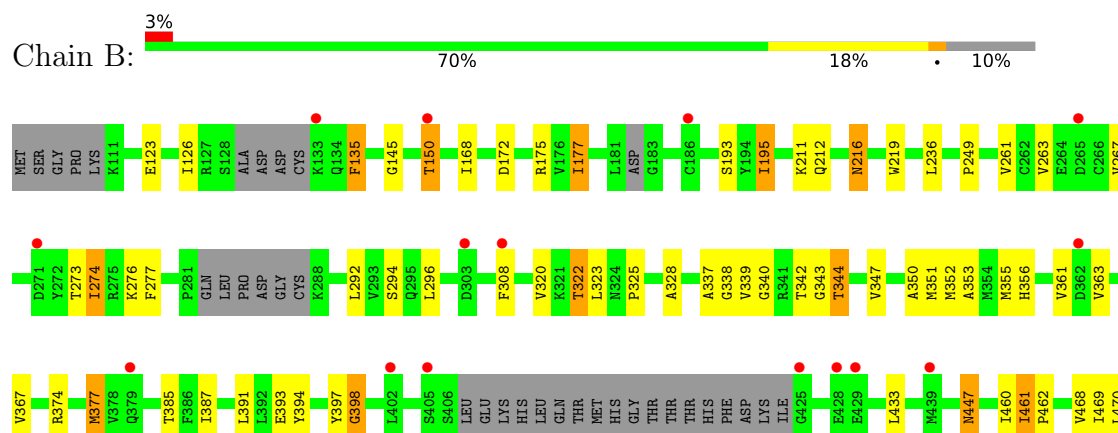
3 Residue-property plots [i](#)

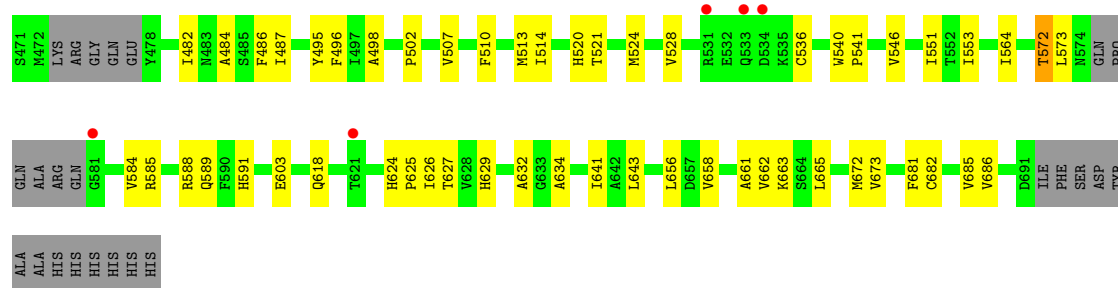
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RECEPTOR-TYPE TYROSINE-PROTEIN PHOSPHATASE EPSILON

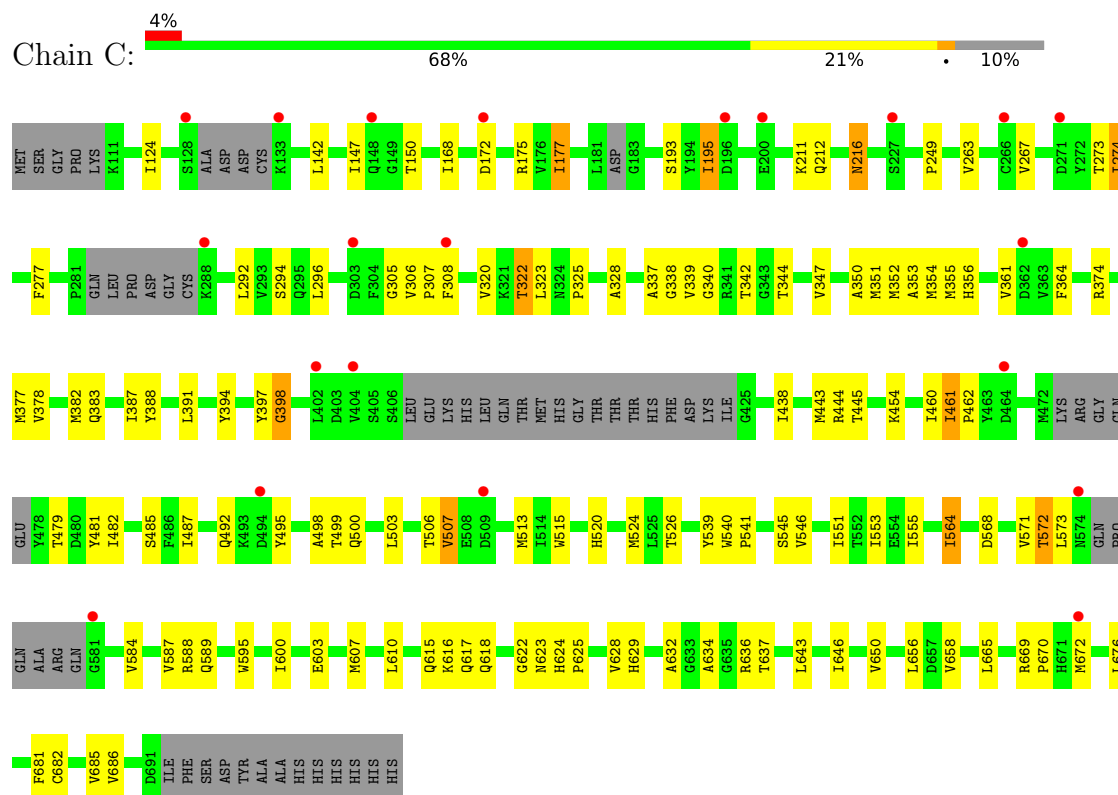


• Molecule 1: RECEPTOR-TYPE TYROSINE-PROTEIN PHOSPHATASE EPSILON

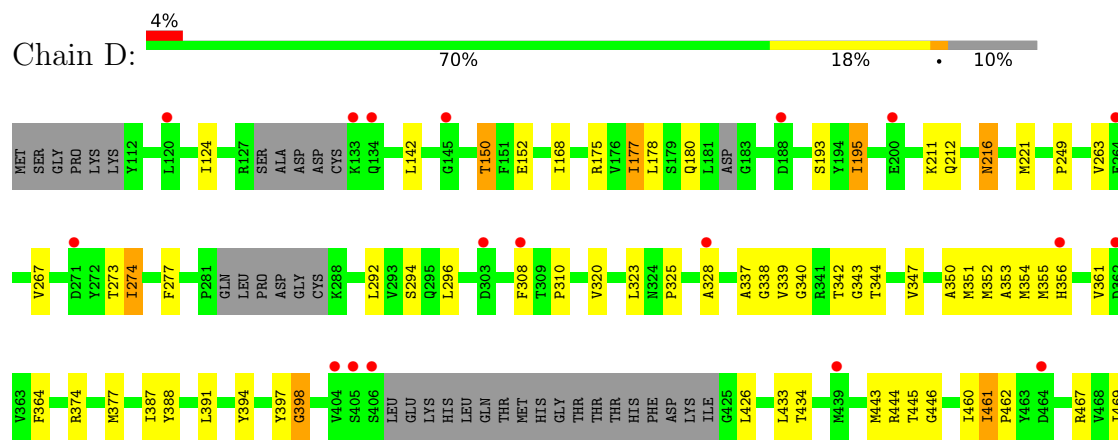


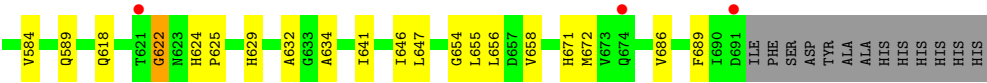


• Molecule 1: RECEPTOR-TYPE TYROSINE-PROTEIN PHOSPHATASE EPSILON



• Molecule 1: RECEPTOR-TYPE TYROSINE-PROTEIN PHOSPHATASE EPSILON





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.02Å 123.62Å 219.12Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	218.22 – 3.20 218.22 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (218.22-3.20) 98.7 (218.22-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.221 , 0.256 0.226 , 0.259	Depositor DCC
R_{free} test set	5498 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 94.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l 0.027 for -k,-h,-l 0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23750	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.66	0/4072	0.84	1/5570 (0.0%)
1	B	0.65	0/4074	0.84	1/5575 (0.0%)
1	C	0.65	0/4071	0.83	2/5570 (0.0%)
1	D	0.61	0/4036	0.80	0/5522
1	E	0.65	0/4051	0.84	2/5544 (0.0%)
1	F	0.64	0/4037	0.83	0/5525
All	All	0.64	0/24341	0.83	6/33306 (0.0%)

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	C	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	VAL	N-CA-C	-8.84	97.19	109.21
1	E	605	LYS	N-CA-C	-6.65	103.73	110.97
1	B	673	VAL	N-CA-C	-5.85	101.16	108.89
1	E	492	GLN	N-CA-C	5.46	117.37	109.07
1	C	492	GLN	N-CA-C	5.30	117.32	108.99
1	C	481	TYR	N-CA-C	5.17	117.16	108.73

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	622	GLY	Peptide
1	F	622	GLY	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	3973	0	3575	104	0
1	B	3972	0	3557	84	0
1	C	3970	0	3551	106	0
1	D	3936	0	3491	90	0
1	E	3950	0	3506	73	0
1	F	3937	0	3491	78	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
All	All	23750	0	21171	531	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 12.

All (531) 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:E:656:LEU:HD11	1:E:686:VAL:HG11	1.27	1.17
1:C:656:LEU:CD1	1:C:686:VAL:HG11	1.86	1.05
1:D:351:MET:HE1	1:D:354:MET:HE3	1.33	1.03
1:D:656:LEU:HD11	1:D:686:VAL:HG11	1.41	1.02
1:F:656:LEU:HD11	1:F:686:VAL:HG11	1.46	0.97
1:C:564:ILE:HG21	1:C:610:LEU:HD13	1.44	0.96
1:A:393:GLU:OE2	1:A:663:LYS:NZ	1.98	0.95
1:C:665:LEU:HD22	1:C:672:MET:HE3	1.45	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:LEU:HD11	1:A:686:VAL:HG11	1.47	0.95
1:B:656:LEU:CD1	1:B:686:VAL:HG11	1.98	0.91
1:C:656:LEU:HD12	1:C:686:VAL:HG11	1.54	0.90
1:E:656:LEU:HD11	1:E:686:VAL:CG1	2.01	0.89
1:A:355:MET:HE3	1:A:391:LEU:HD22	1.55	0.88
1:D:355:MET:HE3	1:D:391:LEU:HD22	1.56	0.88
1:C:564:ILE:CG2	1:C:610:LEU:HD13	2.02	0.88
1:C:665:LEU:HD22	1:C:672:MET:CE	2.03	0.88
1:E:355:MET:HE3	1:E:391:LEU:HD22	1.55	0.88
1:C:355:MET:HE3	1:C:391:LEU:HD22	1.55	0.87
1:D:524:MET:HE2	1:D:589:GLN:NE2	1.89	0.87
1:B:355:MET:HE3	1:B:391:LEU:HD22	1.54	0.86
1:B:656:LEU:HD11	1:B:686:VAL:HG11	1.56	0.86
1:D:351:MET:HE1	1:D:354:MET:CE	2.04	0.86
1:F:355:MET:HE3	1:F:391:LEU:HD22	1.56	0.85
1:E:551:ILE:HD13	1:E:573:LEU:HD13	1.59	0.85
1:C:551:ILE:HD13	1:C:573:LEU:HD13	1.59	0.85
1:B:524:MET:HE2	1:B:589:GLN:NE2	1.93	0.83
1:D:351:MET:CE	1:D:354:MET:HE3	2.08	0.83
1:E:634:ALA:HB1	1:E:672:MET:HA	1.59	0.83
1:E:624:HIS:HB3	1:E:625:PRO:HD2	1.59	0.82
1:C:656:LEU:HD11	1:C:686:VAL:HG11	1.61	0.81
1:B:340:GLY:O	1:B:344:THR:HG23	1.81	0.80
1:E:339:VAL:HG13	1:E:374:ARG:HH11	1.46	0.80
1:A:153:LEU:HD13	1:A:175:ARG:NH1	1.97	0.79
1:B:541:PRO:HB3	1:B:546:VAL:HG13	1.63	0.79
1:B:634:ALA:HB1	1:B:672:MET:HA	1.65	0.79
1:D:361:VAL:HG21	1:D:391:LEU:HD13	1.65	0.78
1:D:665:LEU:HD22	1:D:672:MET:CE	2.13	0.78
1:F:656:LEU:CD1	1:F:686:VAL:HG11	2.13	0.77
1:A:524:MET:HG3	1:A:629:HIS:CE1	2.19	0.77
1:D:340:GLY:O	1:D:344:THR:HG23	1.85	0.76
1:F:524:MET:HE2	1:F:589:GLN:NE2	2.00	0.76
1:C:681:PHE:O	1:C:685:VAL:HG23	1.86	0.76
1:D:551:ILE:HD13	1:D:573:LEU:HD13	1.66	0.75
1:B:524:MET:HG3	1:B:629:HIS:NE2	2.01	0.74
1:F:495:TYR:OH	1:F:618:GLN:HG2	1.88	0.74
1:C:351:MET:HE1	1:C:354:MET:HE3	1.69	0.74
1:D:521:THR:HB	1:D:626:ILE:HG23	1.69	0.73
1:C:339:VAL:HG13	1:C:374:ARG:HH11	1.53	0.73
1:D:656:LEU:CD1	1:D:686:VAL:HG11	2.17	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD12	1:B:377:MET:HE2	1.71	0.73
1:B:123:GLU:HA	1:B:126:ILE:HD12	1.72	0.72
1:F:351:MET:HE1	1:F:354:MET:HE3	1.70	0.72
1:E:340:GLY:O	1:E:344:THR:HG23	1.90	0.71
1:A:338:GLY:C	1:A:342:THR:HG21	2.15	0.71
1:A:524:MET:HE1	1:A:540:TRP:CZ3	2.25	0.71
1:F:634:ALA:HB1	1:F:672:MET:HA	1.71	0.71
1:B:361:VAL:HG21	1:B:391:LEU:HD13	1.72	0.71
1:B:393:GLU:OE2	1:B:663:LYS:NZ	2.24	0.71
1:A:443:MET:HE3	1:A:461:ILE:HG22	1.71	0.70
1:C:524:MET:HE1	1:C:540:TRP:CH2	2.26	0.70
1:B:624:HIS:HB3	1:B:625:PRO:HD2	1.72	0.70
1:B:551:ILE:HD13	1:B:573:LEU:HD13	1.74	0.69
1:E:150:THR:HG22	1:E:172:ASP:OD2	1.92	0.69
1:B:338:GLY:C	1:B:342:THR:HG21	2.17	0.69
1:C:551:ILE:CD1	1:C:573:LEU:HD13	2.22	0.69
1:C:551:ILE:HD13	1:C:573:LEU:CD1	2.23	0.68
1:B:195:ILE:CD1	1:B:377:MET:HE2	2.23	0.68
1:B:150:THR:HG22	1:B:172:ASP:OD2	1.93	0.67
1:C:325:PRO:HG2	1:C:328:ALA:HB2	1.75	0.67
1:E:656:LEU:CD1	1:E:686:VAL:HG11	2.16	0.67
1:F:572:THR:HG23	1:F:584:VAL:HG23	1.77	0.67
1:F:338:GLY:C	1:F:342:THR:HG21	2.18	0.67
1:F:325:PRO:HG2	1:F:328:ALA:HB2	1.77	0.67
1:B:325:PRO:HG2	1:B:328:ALA:HB2	1.76	0.67
1:D:624:HIS:HB3	1:D:625:PRO:HD2	1.76	0.67
1:B:524:MET:HG3	1:B:629:HIS:HE2	1.60	0.67
1:F:347:VAL:HG11	1:F:387:ILE:HD13	1.76	0.67
1:F:524:MET:HE1	1:F:540:TRP:CH2	2.30	0.67
1:A:624:HIS:HB3	1:A:625:PRO:HD2	1.77	0.67
1:D:338:GLY:C	1:D:342:THR:HG21	2.20	0.67
1:D:656:LEU:HD11	1:D:686:VAL:CG1	2.23	0.67
1:F:487:ILE:HD13	1:F:672:MET:HE2	1.77	0.67
1:A:524:MET:HE1	1:A:540:TRP:CH2	2.29	0.66
1:D:325:PRO:HG2	1:D:328:ALA:HB2	1.75	0.66
1:F:153:LEU:HD13	1:F:175:ARG:NH1	2.09	0.66
1:C:338:GLY:C	1:C:342:THR:HG21	2.20	0.66
1:E:338:GLY:C	1:E:342:THR:HG21	2.20	0.66
1:F:624:HIS:HB3	1:F:625:PRO:HD2	1.77	0.66
1:F:641:ILE:HD12	1:F:672:MET:HE1	1.78	0.66
1:F:150:THR:HG22	1:F:172:ASP:OD2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:461:ILE:HG23	1:F:462:PRO:HD2	1.79	0.65
1:C:443:MET:CE	1:C:461:ILE:HG22	2.27	0.65
1:A:153:LEU:HD13	1:A:175:ARG:HH11	1.62	0.65
1:D:460:ILE:HD12	1:D:632:ALA:HB1	1.77	0.65
1:E:325:PRO:HG2	1:E:328:ALA:HB2	1.78	0.64
1:E:347:VAL:HG11	1:E:387:ILE:HD13	1.79	0.64
1:A:325:PRO:HG2	1:A:328:ALA:HB2	1.77	0.64
1:A:347:VAL:HG11	1:A:387:ILE:HD13	1.78	0.64
1:D:487:ILE:HD12	1:D:498:ALA:HB2	1.79	0.64
1:D:618:GLN:NE2	1:D:626:ILE:HG12	2.12	0.63
1:A:343:GLY:HA2	1:A:377:MET:HE3	1.81	0.63
1:A:624:HIS:HB3	1:A:625:PRO:CD	2.28	0.63
1:C:361:VAL:HG21	1:C:391:LEU:HD13	1.81	0.63
1:C:515:TRP:NE1	1:C:573:LEU:HD22	2.14	0.63
1:C:564:ILE:HG21	1:C:610:LEU:CD1	2.23	0.63
1:A:402:LEU:HD23	1:A:656:LEU:HB3	1.81	0.62
1:B:296:LEU:HD13	1:B:320:VAL:HG22	1.80	0.62
1:B:460:ILE:HD12	1:B:632:ALA:HB1	1.80	0.62
1:F:339:VAL:HG13	1:F:374:ARG:HH11	1.63	0.62
1:B:347:VAL:HG11	1:B:387:ILE:HD13	1.80	0.62
1:B:528:VAL:HG13	1:B:536:CYS:O	1.99	0.62
1:D:296:LEU:HD13	1:D:320:VAL:HG22	1.81	0.62
1:B:487:ILE:HD13	1:B:672:MET:HE2	1.81	0.62
1:C:545:SER:HA	1:C:553:ILE:O	2.00	0.62
1:C:634:ALA:HB1	1:C:672:MET:HA	1.81	0.62
1:B:343:GLY:HA2	1:B:377:MET:HE3	1.83	0.61
1:A:680:GLU:HG2	1:C:147:ILE:HD12	1.82	0.61
1:D:347:VAL:HG11	1:D:387:ILE:HD13	1.83	0.61
1:C:168:ILE:HD13	1:C:337:ALA:HB1	1.82	0.61
1:C:347:VAL:HG11	1:C:387:ILE:HD13	1.81	0.61
1:D:249:PRO:HG2	1:D:263:VAL:HG23	1.82	0.61
1:D:524:MET:HG3	1:D:629:HIS:NE2	2.16	0.61
1:E:551:ILE:CD1	1:E:573:LEU:HD13	2.28	0.60
1:C:520:HIS:HA	1:C:587:VAL:HG22	1.83	0.60
1:C:524:MET:HE1	1:C:540:TRP:CZ3	2.36	0.60
1:D:524:MET:HE1	1:D:540:TRP:CH2	2.37	0.60
1:E:296:LEU:HD13	1:E:320:VAL:HG22	1.84	0.60
1:B:168:ILE:HD13	1:B:337:ALA:HB1	1.82	0.60
1:B:461:ILE:HG23	1:B:462:PRO:HD2	1.82	0.60
1:B:249:PRO:HG2	1:B:263:VAL:HG23	1.83	0.60
1:E:564:ILE:HG21	1:E:610:LEU:HD13	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PRO:HG2	1:A:263:VAL:HG23	1.84	0.60
1:A:524:MET:HG3	1:A:629:HIS:NE2	2.17	0.60
1:E:249:PRO:HG2	1:E:263:VAL:HG23	1.82	0.60
1:A:487:ILE:HD13	1:A:672:MET:HE2	1.83	0.59
1:A:433:LEU:CD1	1:A:662:VAL:HG11	2.31	0.59
1:B:502:PRO:HG3	1:B:510:PHE:CD1	2.36	0.59
1:E:665:LEU:HD22	1:E:672:MET:CE	2.33	0.59
1:C:628:VAL:CG1	1:C:637:THR:HG23	2.33	0.59
1:A:338:GLY:O	1:A:342:THR:HG21	2.01	0.59
1:A:635:GLY:N	1:A:672:MET:O	2.36	0.59
1:D:665:LEU:HD22	1:D:672:MET:HE2	1.82	0.59
1:F:168:ILE:HD13	1:F:337:ALA:HB1	1.85	0.59
1:A:665:LEU:HD22	1:A:672:MET:HE3	1.84	0.58
1:D:551:ILE:CD1	1:D:573:LEU:HD13	2.32	0.58
1:F:296:LEU:HD13	1:F:320:VAL:HG22	1.85	0.58
1:F:249:PRO:HG2	1:F:263:VAL:HG23	1.85	0.58
1:D:124:ILE:CD1	1:D:388:TYR:HB3	2.34	0.58
1:E:175:ARG:NH2	1:E:177:ILE:HG22	2.19	0.58
1:B:572:THR:HG23	1:B:584:VAL:HG23	1.85	0.58
1:C:443:MET:HE3	1:C:461:ILE:HG22	1.85	0.58
1:C:249:PRO:HG2	1:C:263:VAL:HG23	1.86	0.58
1:D:487:ILE:HD13	1:D:672:MET:CE	2.33	0.58
1:B:175:ARG:NH2	1:B:177:ILE:HG22	2.19	0.57
1:C:306:VAL:HG13	1:C:382:MET:HG2	1.86	0.57
1:A:461:ILE:HG23	1:A:462:PRO:HD2	1.85	0.57
1:C:340:GLY:O	1:C:344:THR:HG23	2.03	0.57
1:C:541:PRO:HB3	1:C:546:VAL:HG13	1.85	0.57
1:D:175:ARG:NH2	1:D:177:ILE:HG22	2.19	0.57
1:D:634:ALA:HB1	1:D:672:MET:HA	1.85	0.57
1:A:296:LEU:HD13	1:A:320:VAL:HG22	1.87	0.57
1:E:624:HIS:HB3	1:E:625:PRO:CD	2.33	0.57
1:E:681:PHE:O	1:E:685:VAL:HG23	2.05	0.57
1:C:175:ARG:NH2	1:C:177:ILE:HG22	2.20	0.57
1:E:487:ILE:HD13	1:E:672:MET:HE2	1.86	0.57
1:A:168:ILE:HD13	1:A:337:ALA:HB1	1.87	0.56
1:D:654:GLY:O	1:D:655:LEU:HD23	2.04	0.56
1:E:361:VAL:HG21	1:E:391:LEU:HD13	1.87	0.56
1:E:524:MET:HG3	1:E:629:HIS:CE1	2.40	0.56
1:C:595:TRP:CZ3	1:C:607:MET:HE1	2.40	0.56
1:C:553:ILE:HD13	1:C:571:VAL:HG13	1.88	0.56
1:F:646:ILE:HD13	1:F:658:VAL:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:GLN:NE2	1:B:624:HIS:O	2.39	0.56
1:D:515:TRP:NE1	1:D:573:LEU:HD22	2.21	0.56
1:F:175:ARG:NH2	1:F:177:ILE:HG22	2.21	0.56
1:B:447:ASN:N	1:B:447:ASN:HD22	2.03	0.56
1:E:168:ILE:HD13	1:E:337:ALA:HB1	1.86	0.56
1:E:524:MET:HE2	1:E:589:GLN:NE2	2.20	0.56
1:A:495:TYR:OH	1:A:618:GLN:HG2	2.06	0.56
1:A:515:TRP:NE1	1:A:573:LEU:HD22	2.21	0.55
1:A:322:THR:HG22	1:A:323:LEU:HD23	1.87	0.55
1:C:296:LEU:HD13	1:C:320:VAL:HG22	1.87	0.55
1:A:175:ARG:NH2	1:A:177:ILE:HG22	2.21	0.55
1:A:402:LEU:CD2	1:A:656:LEU:HD22	2.37	0.55
1:D:168:ILE:HD13	1:D:337:ALA:HB1	1.89	0.55
1:D:620:GLN:C	1:D:622:GLY:H	2.14	0.55
1:A:468:VAL:HG11	1:A:513:MET:HG3	1.87	0.55
1:A:520:HIS:NE2	1:A:585:ARG:HD3	2.22	0.54
1:B:468:VAL:HG22	1:B:486:PHE:CE2	2.43	0.54
1:C:524:MET:HG3	1:C:629:HIS:CE1	2.43	0.54
1:A:499:THR:HG23	1:A:629:HIS:HB3	1.90	0.54
1:F:211:LYS:O	1:F:212:GLN:C	2.51	0.54
1:C:682:CYS:O	1:C:686:VAL:HG23	2.07	0.54
1:C:628:VAL:HG12	1:C:637:THR:HG23	1.90	0.54
1:B:469:ILE:O	1:B:470:LEU:HD23	2.08	0.54
1:E:524:MET:HG3	1:E:629:HIS:NE2	2.22	0.54
1:A:665:LEU:HD22	1:A:672:MET:CE	2.36	0.54
1:E:515:TRP:NE1	1:E:573:LEU:HD22	2.23	0.54
1:E:665:LEU:HD22	1:E:672:MET:HE2	1.90	0.54
1:B:338:GLY:O	1:B:342:THR:HG21	2.08	0.54
1:A:150:THR:HG22	1:A:172:ASP:CG	2.33	0.53
1:A:361:VAL:HG21	1:A:391:LEU:HD13	1.90	0.53
1:F:274:ILE:CG2	1:F:274:ILE:O	2.57	0.53
1:F:528:VAL:HG13	1:F:536:CYS:O	2.09	0.53
1:C:495:TYR:OH	1:C:618:GLN:HG2	2.09	0.53
1:B:322:THR:HG22	1:B:323:LEU:HD23	1.90	0.53
1:D:274:ILE:O	1:D:274:ILE:CG2	2.57	0.53
1:B:495:TYR:OH	1:B:618:GLN:HG2	2.08	0.53
1:C:374:ARG:O	1:C:377:MET:HG2	2.08	0.53
1:D:274:ILE:HD11	1:D:323:LEU:HD11	1.90	0.53
1:F:401:GLU:HA	1:F:656:LEU:O	2.09	0.53
1:F:502:PRO:HG3	1:F:510:PHE:CD1	2.43	0.53
1:B:211:LYS:O	1:B:212:GLN:C	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:THR:HG22	1:C:323:LEU:HD23	1.91	0.52
1:C:438:ILE:HD13	1:C:670:PRO:CB	2.39	0.52
1:A:502:PRO:HG3	1:A:510:PHE:CD1	2.43	0.52
1:A:656:LEU:CD1	1:A:686:VAL:HG11	2.31	0.52
1:D:682:CYS:O	1:D:686:VAL:HG23	2.10	0.52
1:F:267:VAL:HB	1:F:274:ILE:HG22	1.90	0.52
1:F:515:TRP:NE1	1:F:573:LEU:HD22	2.24	0.52
1:C:274:ILE:O	1:C:274:ILE:CG2	2.58	0.52
1:D:469:ILE:C	1:D:470:LEU:HD23	2.35	0.52
1:C:195:ILE:CD1	1:C:377:MET:HE2	2.40	0.52
1:C:487:ILE:HD13	1:C:672:MET:CE	2.40	0.52
1:B:681:PHE:O	1:B:685:VAL:HG23	2.10	0.52
1:F:524:MET:HG3	1:F:629:HIS:NE2	2.24	0.52
1:A:340:GLY:O	1:A:344:THR:HG23	2.09	0.52
1:F:397:TYR:O	1:F:398:GLY:C	2.52	0.52
1:C:344:THR:HG21	1:C:383:GLN:HG2	1.92	0.52
1:A:426:LEU:H	1:A:426:LEU:HD12	1.75	0.51
1:A:611:ILE:HD13	1:A:647:LEU:HD12	1.93	0.51
1:E:524:MET:HE1	1:E:540:TRP:CH2	2.45	0.51
1:A:277:PHE:O	1:A:292:LEU:HD23	2.10	0.51
1:C:351:MET:HE1	1:C:354:MET:CE	2.38	0.51
1:D:665:LEU:HD22	1:D:672:MET:HE3	1.91	0.51
1:A:487:ILE:CD1	1:A:672:MET:HE2	2.40	0.51
1:E:355:MET:HE3	1:E:391:LEU:CD2	2.36	0.51
1:A:354:MET:HE3	1:A:358:GLU:OE2	2.11	0.51
1:A:487:ILE:HD12	1:A:498:ALA:HB2	1.92	0.51
1:C:338:GLY:O	1:C:342:THR:HG21	2.10	0.51
1:A:433:LEU:HD11	1:A:662:VAL:HG11	1.91	0.51
1:C:460:ILE:HD12	1:C:632:ALA:HB1	1.92	0.51
1:A:153:LEU:HD22	1:A:175:ARG:CZ	2.41	0.51
1:D:564:ILE:HG21	1:D:610:LEU:HD13	1.92	0.51
1:E:503:LEU:HD13	1:E:505:HIS:HE1	1.75	0.51
1:A:460:ILE:HD12	1:A:632:ALA:HB1	1.93	0.51
1:B:351:MET:HA	1:B:351:MET:HE2	1.93	0.51
1:D:443:MET:HE3	1:D:461:ILE:HG22	1.93	0.51
1:F:654:GLY:O	1:F:655:LEU:HD23	2.10	0.51
1:A:217:ASP:N	1:A:217:ASP:OD2	2.44	0.50
1:A:524:MET:CE	1:A:589:GLN:NE2	2.74	0.50
1:D:564:ILE:CG2	1:D:610:LEU:HD13	2.40	0.50
1:E:343:GLY:HA2	1:E:377:MET:HE3	1.93	0.50
1:C:277:PHE:O	1:C:292:LEU:HD23	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LYS:O	1:E:212:GLN:C	2.54	0.50
1:A:487:ILE:HG21	1:A:641:ILE:HG21	1.94	0.50
1:B:274:ILE:HD11	1:B:323:LEU:HD11	1.92	0.50
1:E:461:ILE:HG23	1:E:462:PRO:HD2	1.94	0.50
1:F:456:ARG:NH2	1:F:536:CYS:HA	2.27	0.50
1:A:239:ARG:O	1:A:240:LYS:CB	2.60	0.50
1:A:370:ILE:HD12	1:A:377:MET:HG3	1.94	0.50
1:B:274:ILE:O	1:B:274:ILE:CG2	2.60	0.50
1:B:524:MET:HE3	1:B:591:HIS:CG	2.47	0.50
1:B:355:MET:HE3	1:B:391:LEU:CD2	2.35	0.50
1:F:618:GLN:O	1:F:622:GLY:HA2	2.11	0.50
1:B:363:VAL:O	1:B:367:VAL:HG23	2.12	0.50
1:C:355:MET:HE3	1:C:391:LEU:CD2	2.35	0.50
1:D:267:VAL:HB	1:D:274:ILE:HG22	1.94	0.50
1:E:274:ILE:O	1:E:274:ILE:CG2	2.60	0.50
1:A:274:ILE:HD11	1:A:323:LEU:HD11	1.93	0.50
1:C:487:ILE:HD13	1:C:672:MET:HE1	1.92	0.49
1:E:690:ILE:HG22	1:E:690:ILE:O	2.12	0.49
1:F:274:ILE:HD11	1:F:323:LEU:HD11	1.94	0.49
1:F:343:GLY:HA2	1:F:377:MET:HE3	1.94	0.49
1:A:144:SER:O	1:A:146:HIS:N	2.43	0.49
1:C:443:MET:HE2	1:C:461:ILE:HG22	1.94	0.49
1:D:495:TYR:OH	1:D:618:GLN:HG2	2.13	0.49
1:E:267:VAL:HB	1:E:274:ILE:HG22	1.94	0.49
1:E:338:GLY:O	1:E:342:THR:HG21	2.12	0.49
1:F:552:THR:C	1:F:553:ILE:HD13	2.38	0.49
1:C:524:MET:HG3	1:C:629:HIS:NE2	2.26	0.49
1:A:267:VAL:HB	1:A:274:ILE:HG22	1.94	0.49
1:C:461:ILE:HG23	1:C:462:PRO:HD2	1.94	0.49
1:C:624:HIS:HB3	1:C:625:PRO:HD2	1.94	0.49
1:D:340:GLY:N	1:D:377:MET:O	2.46	0.49
1:A:211:LYS:O	1:A:212:GLN:C	2.54	0.49
1:A:352:MET:HE3	1:A:394:TYR:CE1	2.47	0.49
1:D:635:GLY:N	1:D:672:MET:O	2.45	0.49
1:A:656:LEU:HD21	1:A:658:VAL:HG23	1.95	0.49
1:F:351:MET:HE1	1:F:354:MET:CE	2.39	0.49
1:A:541:PRO:HB3	1:A:546:VAL:HG13	1.94	0.49
1:A:618:GLN:O	1:A:622:GLY:HA2	2.13	0.48
1:E:274:ILE:HD11	1:E:323:LEU:HD11	1.94	0.48
1:C:305:GLY:HA2	1:C:382:MET:HE3	1.94	0.48
1:A:195:ILE:HD12	1:A:377:MET:HE2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ARG:O	1:A:637:THR:C	2.55	0.48
1:E:690:ILE:O	1:E:690:ILE:CG2	2.61	0.48
1:F:551:ILE:CD1	1:F:573:LEU:HD13	2.44	0.48
1:B:352:MET:HE3	1:B:394:TYR:CE1	2.49	0.48
1:D:444:ARG:O	1:D:445:THR:C	2.55	0.48
1:F:656:LEU:HD21	1:F:658:VAL:HG23	1.95	0.48
1:C:487:ILE:HD12	1:C:498:ALA:HB2	1.95	0.48
1:D:277:PHE:O	1:D:292:LEU:HD23	2.14	0.48
1:E:666:ARG:NH2	1:E:673:VAL:O	2.46	0.48
1:A:479:THR:O	1:A:479:THR:HG22	2.14	0.48
1:A:666:ARG:NH2	1:A:673:VAL:O	2.46	0.48
1:D:339:VAL:HG13	1:D:374:ARG:HH11	1.78	0.48
1:B:374:ARG:O	1:B:377:MET:HG2	2.14	0.48
1:A:402:LEU:HD21	1:A:656:LEU:HD13	1.96	0.48
1:B:487:ILE:HD12	1:B:498:ALA:CB	2.44	0.48
1:C:495:TYR:O	1:C:625:PRO:HA	2.13	0.48
1:E:339:VAL:HG13	1:E:374:ARG:NH1	2.23	0.48
1:A:433:LEU:CD1	1:A:662:VAL:CG1	2.91	0.48
1:D:487:ILE:HD12	1:D:498:ALA:CB	2.43	0.47
1:D:643:LEU:HD21	1:D:682:CYS:HA	1.95	0.47
1:E:502:PRO:HG3	1:E:510:PHE:CD1	2.48	0.47
1:D:541:PRO:HB3	1:D:546:VAL:HG13	1.96	0.47
1:A:641:ILE:CG2	1:A:665:LEU:HD21	2.45	0.47
1:C:646:ILE:O	1:C:650:VAL:HG23	2.14	0.47
1:D:446:GLY:HA3	1:D:461:ILE:HD13	1.97	0.47
1:D:469:ILE:O	1:D:470:LEU:HD23	2.14	0.47
1:C:150:THR:HG22	1:C:172:ASP:OD2	2.14	0.47
1:A:524:MET:CE	1:A:540:TRP:CZ3	2.97	0.47
1:B:524:MET:HG3	1:B:629:HIS:CE1	2.50	0.47
1:D:524:MET:CE	1:D:589:GLN:NE2	2.71	0.47
1:B:277:PHE:O	1:B:292:LEU:HD23	2.15	0.47
1:A:216:ASN:HD22	1:A:216:ASN:N	2.12	0.47
1:C:274:ILE:HD11	1:C:323:LEU:HD11	1.97	0.47
1:D:568:ASP:OD1	1:D:588:ARG:HD2	2.15	0.47
1:D:646:ILE:O	1:D:650:VAL:HG23	2.14	0.47
1:E:528:VAL:HG13	1:E:536:CYS:O	2.14	0.47
1:F:524:MET:HG3	1:F:629:HIS:CE1	2.49	0.47
1:C:216:ASN:N	1:C:216:ASN:HD22	2.13	0.47
1:F:374:ARG:O	1:F:377:MET:HG2	2.15	0.47
1:A:343:GLY:CA	1:A:377:MET:HE3	2.45	0.47
1:A:520:HIS:HE2	1:A:585:ARG:HD3	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:ILE:HD13	1:C:658:VAL:HG22	1.97	0.47
1:D:211:LYS:O	1:D:212:GLN:C	2.58	0.47
1:A:351:MET:HE2	1:A:351:MET:HA	1.97	0.46
1:A:634:ALA:HB1	1:A:672:MET:HA	1.97	0.46
1:E:216:ASN:N	1:E:216:ASN:HD22	2.13	0.46
1:F:338:GLY:O	1:F:342:THR:HG21	2.15	0.46
1:A:526:THR:HG22	1:A:636:ARG:NH1	2.30	0.46
1:D:426:LEU:HD12	1:D:426:LEU:N	2.30	0.46
1:F:541:PRO:HB3	1:F:546:VAL:HG13	1.97	0.46
1:A:433:LEU:HD11	1:A:662:VAL:CG1	2.46	0.46
1:C:211:LYS:O	1:C:212:GLN:C	2.58	0.46
1:C:352:MET:HE3	1:C:394:TYR:CE1	2.49	0.46
1:F:461:ILE:HG23	1:F:462:PRO:CD	2.44	0.46
1:F:656:LEU:C	1:F:656:LEU:HD23	2.41	0.46
1:F:124:ILE:CD1	1:F:388:TYR:HB3	2.46	0.46
1:C:351:MET:HE2	1:C:351:MET:HA	1.98	0.46
1:B:267:VAL:HB	1:B:274:ILE:HG22	1.96	0.46
1:E:656:LEU:CD1	1:E:686:VAL:CG1	2.85	0.46
1:C:274:ILE:O	1:C:274:ILE:HG22	2.16	0.46
1:C:444:ARG:O	1:C:445:THR:C	2.59	0.46
1:A:555:ILE:HG23	1:A:555:ILE:O	2.16	0.46
1:B:520:HIS:NE2	1:B:585:ARG:HD3	2.30	0.46
1:C:438:ILE:HD13	1:C:670:PRO:HB2	1.98	0.46
1:D:338:GLY:O	1:D:342:THR:HG21	2.14	0.46
1:F:239:ARG:O	1:F:240:LYS:CB	2.63	0.46
1:A:564:ILE:HD13	1:A:564:ILE:N	2.31	0.46
1:A:641:ILE:HG22	1:A:665:LEU:HD21	1.97	0.46
1:D:564:ILE:HG21	1:D:610:LEU:CD1	2.45	0.46
1:B:524:MET:HE1	1:B:540:TRP:CH2	2.50	0.46
1:D:487:ILE:HD13	1:D:672:MET:HE1	1.96	0.46
1:C:124:ILE:CD1	1:C:388:TYR:HB3	2.46	0.45
1:E:277:PHE:O	1:E:292:LEU:HD23	2.15	0.45
1:E:601:PRO:HG2	1:E:681:PHE:CZ	2.50	0.45
1:F:460:ILE:HD12	1:F:632:ALA:HB1	1.98	0.45
1:A:524:MET:HE3	1:A:589:GLN:NE2	2.31	0.45
1:B:433:LEU:HD13	1:B:662:VAL:HG11	1.98	0.45
1:D:443:MET:CE	1:D:461:ILE:HG22	2.46	0.45
1:B:521:THR:HB	1:B:626:ILE:HG23	1.98	0.45
1:C:503:LEU:HB2	1:C:506:THR:HG23	1.96	0.45
1:D:142:LEU:HD23	1:D:364:PHE:CE1	2.50	0.45
1:C:568:ASP:OD1	1:C:588:ARG:HD3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:647:LEU:O	1:D:648:GLU:C	2.58	0.45
1:F:352:MET:HE3	1:F:394:TYR:CE1	2.52	0.45
1:D:274:ILE:O	1:D:274:ILE:HG22	2.16	0.45
1:D:397:TYR:O	1:D:398:GLY:C	2.59	0.45
1:E:495:TYR:OH	1:E:618:GLN:HG2	2.17	0.45
1:A:175:ARG:CZ	1:A:177:ILE:HG22	2.47	0.45
1:B:216:ASN:N	1:B:216:ASN:HD22	2.14	0.45
1:A:515:TRP:CE2	1:A:573:LEU:HD22	2.52	0.45
1:B:219:TRP:CE2	1:B:261:VAL:HG21	2.52	0.45
1:C:142:LEU:HD23	1:C:364:PHE:CE1	2.52	0.45
1:E:397:TYR:O	1:E:398:GLY:C	2.59	0.45
1:F:361:VAL:HG21	1:F:391:LEU:HD13	1.99	0.45
1:D:434:THR:O	1:D:434:THR:HG22	2.16	0.45
1:B:524:MET:HE2	1:B:589:GLN:HE21	1.75	0.45
1:C:485:SER:HB2	1:C:669:ARG:HD2	1.98	0.45
1:C:616:LYS:O	1:C:617:GLN:C	2.60	0.45
1:F:150:THR:CG2	1:F:172:ASP:OD2	2.63	0.45
1:F:153:LEU:HD22	1:F:175:ARG:CZ	2.47	0.45
1:A:566:ILE:O	1:A:566:ILE:HG22	2.16	0.44
1:B:274:ILE:O	1:B:274:ILE:HG22	2.18	0.44
1:D:676:LEU:HD12	1:D:676:LEU:O	2.18	0.44
1:B:643:LEU:HD11	1:B:685:VAL:HG21	1.99	0.44
1:D:351:MET:HA	1:D:351:MET:HE2	1.99	0.44
1:D:524:MET:HE2	1:D:589:GLN:HE22	1.75	0.44
1:E:487:ILE:HD12	1:E:498:ALA:HB2	1.99	0.44
1:F:274:ILE:O	1:F:274:ILE:HG22	2.17	0.44
1:B:624:HIS:HB3	1:B:625:PRO:CD	2.44	0.44
1:A:397:TYR:O	1:A:398:GLY:C	2.61	0.44
1:A:443:MET:HE3	1:A:461:ILE:CG2	2.43	0.44
1:D:624:HIS:HB3	1:D:625:PRO:CD	2.47	0.44
1:B:514:ILE:HD11	1:B:627:THR:HG21	1.98	0.44
1:B:665:LEU:HD22	1:B:672:MET:HE2	1.99	0.44
1:E:355:MET:HE1	1:E:391:LEU:O	2.18	0.44
1:D:526:THR:HG22	1:D:636:ARG:HH11	1.83	0.44
1:B:355:MET:HE1	1:B:391:LEU:O	2.17	0.44
1:E:175:ARG:CZ	1:E:177:ILE:HG22	2.48	0.44
1:A:528:VAL:HG13	1:A:536:CYS:O	2.18	0.44
1:D:216:ASN:N	1:D:216:ASN:HD22	2.15	0.44
1:A:656:LEU:CD2	1:A:658:VAL:HG23	2.47	0.43
1:E:150:THR:CG2	1:E:172:ASP:OD2	2.62	0.43
1:F:495:TYR:O	1:F:625:PRO:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:ILE:CD1	1:C:571:VAL:HG13	2.47	0.43
1:F:277:PHE:O	1:F:292:LEU:HD23	2.19	0.43
1:F:435:ASN:N	1:F:435:ASN:HD22	2.16	0.43
1:A:392:LEU:HD11	1:A:396:LEU:HD21	2.01	0.43
1:E:507:VAL:HG11	1:E:537:TYR:CE2	2.54	0.43
1:A:123:GLU:HA	1:A:126:ILE:HD12	2.00	0.43
1:F:142:LEU:HD23	1:F:364:PHE:CE1	2.54	0.43
1:F:175:ARG:CZ	1:F:177:ILE:HG22	2.48	0.43
1:F:541:PRO:HG3	1:F:546:VAL:HG22	2.00	0.43
1:B:339:VAL:HG13	1:B:374:ARG:HH11	1.84	0.43
1:D:374:ARG:O	1:D:377:MET:HG2	2.18	0.43
1:D:433:LEU:HD13	1:D:662:VAL:HG12	2.00	0.43
1:D:568:ASP:OD1	1:D:588:ARG:CD	2.66	0.43
1:E:662:VAL:HG13	1:E:673:VAL:CG2	2.48	0.43
1:E:482:ILE:HG23	1:E:482:ILE:O	2.18	0.43
1:E:564:ILE:CG2	1:E:610:LEU:HD13	2.47	0.43
1:B:482:ILE:HG23	1:B:484:ALA:HB3	1.99	0.43
1:C:267:VAL:HB	1:C:274:ILE:HG22	1.99	0.43
1:C:344:THR:HG22	1:C:378:VAL:HG13	2.00	0.43
1:C:600:ILE:HD13	1:C:681:PHE:HB2	2.01	0.43
1:D:175:ARG:CZ	1:D:177:ILE:HG22	2.49	0.43
1:F:438:ILE:HD11	1:F:671:HIS:CE1	2.53	0.43
1:A:355:MET:HE3	1:A:391:LEU:CD2	2.36	0.43
1:B:487:ILE:HD13	1:B:672:MET:CE	2.48	0.43
1:C:555:ILE:HG23	1:C:555:ILE:O	2.18	0.43
1:C:607:MET:HE3	1:C:681:PHE:HE2	1.84	0.43
1:E:195:ILE:HD12	1:E:377:MET:HE2	2.01	0.43
1:E:350:ALA:O	1:E:353:ALA:HB3	2.19	0.43
1:E:524:MET:CG	1:E:629:HIS:CE1	3.02	0.43
1:E:555:ILE:HG23	1:E:555:ILE:O	2.19	0.43
1:A:153:LEU:CD1	1:A:175:ARG:NH1	2.76	0.43
1:B:135:PHE:CG	1:B:385:THR:HG22	2.53	0.43
1:C:676:LEU:HD12	1:C:676:LEU:O	2.19	0.43
1:A:471:SER:O	1:A:512:ARG:NH2	2.52	0.42
1:B:524:MET:HE3	1:B:591:HIS:CD2	2.54	0.42
1:C:572:THR:HG23	1:C:584:VAL:HG23	2.01	0.42
1:B:350:ALA:O	1:B:353:ALA:HB3	2.19	0.42
1:E:590:PHE:CD1	1:E:614:VAL:HG22	2.55	0.42
1:F:555:ILE:HG23	1:F:555:ILE:O	2.18	0.42
1:A:426:LEU:HD22	1:C:147:ILE:CD1	2.49	0.42
1:B:524:MET:CG	1:B:629:HIS:CE1	3.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:VAL:HB	1:C:307:PRO:HD2	2.01	0.42
1:D:350:ALA:O	1:D:353:ALA:HB3	2.20	0.42
1:B:487:ILE:HD12	1:B:498:ALA:HB2	2.01	0.42
1:B:643:LEU:HD21	1:B:682:CYS:HA	2.02	0.42
1:C:656:LEU:HD23	1:C:656:LEU:O	2.18	0.42
1:E:113:PHE:CD2	1:E:113:PHE:N	2.88	0.42
1:E:274:ILE:O	1:E:274:ILE:HG22	2.18	0.42
1:E:507:VAL:HG11	1:E:537:TYR:CD2	2.54	0.42
1:A:124:ILE:CD1	1:A:388:TYR:HB3	2.50	0.42
1:A:150:THR:HG22	1:A:172:ASP:HB2	2.02	0.42
1:A:219:TRP:CE2	1:A:261:VAL:HG21	2.54	0.42
1:A:371:ARG:HG2	1:A:377:MET:H	1.83	0.42
1:D:195:ILE:CD1	1:D:377:MET:HE2	2.49	0.42
1:E:178:LEU:HD21	1:E:221:MET:HB2	2.02	0.42
1:F:355:MET:HE1	1:F:391:LEU:O	2.19	0.42
1:F:504:ALA:O	1:F:507:VAL:HG22	2.20	0.42
1:A:347:VAL:CG1	1:A:387:ILE:HD13	2.48	0.42
1:B:276:LYS:HG2	1:C:584:VAL:HG11	2.01	0.42
1:C:175:ARG:CZ	1:C:177:ILE:HG22	2.50	0.42
1:F:553:ILE:HD12	1:F:571:VAL:HG22	2.01	0.42
1:B:658:VAL:O	1:B:661:ALA:HB3	2.20	0.42
1:D:539:TYR:OH	1:D:589:GLN:NE2	2.52	0.42
1:E:618:GLN:O	1:E:622:GLY:HA2	2.20	0.42
1:F:347:VAL:CG1	1:F:387:ILE:HD13	2.47	0.42
1:D:343:GLY:HA2	1:D:377:MET:HE3	2.02	0.41
1:F:551:ILE:HD13	1:F:573:LEU:HD13	2.01	0.41
1:B:397:TYR:O	1:B:398:GLY:C	2.63	0.41
1:C:515:TRP:CE2	1:C:573:LEU:HD22	2.54	0.41
1:C:524:MET:HE2	1:C:589:GLN:NE2	2.35	0.41
1:F:371:ARG:NH2	1:F:378:VAL:O	2.53	0.41
1:F:487:ILE:HD12	1:F:498:ALA:HB2	2.02	0.41
1:F:647:LEU:HD22	1:F:689:PHE:CD2	2.55	0.41
1:B:496:PHE:CE2	1:B:626:ILE:HD12	2.55	0.41
1:C:526:THR:HG22	1:C:636:ARG:NH1	2.35	0.41
1:D:150:THR:HG23	1:D:152:GLU:H	1.85	0.41
1:A:274:ILE:O	1:A:274:ILE:CG2	2.68	0.41
1:C:507:VAL:HG12	1:C:539:TYR:HB3	2.02	0.41
1:A:433:LEU:HD13	1:A:662:VAL:CG1	2.50	0.41
1:C:397:TYR:O	1:C:398:GLY:C	2.63	0.41
1:F:178:LEU:HD21	1:F:221:MET:HB2	2.02	0.41
1:B:175:ARG:CZ	1:B:177:ILE:HG22	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ALA:O	1:C:353:ALA:HB3	2.20	0.41
1:C:482:ILE:HD13	1:C:513:MET:SD	2.61	0.41
1:F:350:ALA:O	1:F:353:ALA:HB3	2.21	0.41
1:B:347:VAL:CG1	1:B:387:ILE:HD13	2.50	0.41
1:C:643:LEU:HD21	1:C:682:CYS:HA	2.02	0.41
1:D:352:MET:HE3	1:D:394:TYR:CE1	2.56	0.41
1:D:570:LEU:HD23	1:D:586:VAL:HG22	2.03	0.41
1:E:124:ILE:CD1	1:E:388:TYR:HB3	2.51	0.41
1:B:482:ILE:HD13	1:B:513:MET:SD	2.60	0.41
1:D:178:LEU:HD21	1:D:221:MET:HB2	2.03	0.41
1:D:195:ILE:HD12	1:D:377:MET:HE2	2.02	0.41
1:B:276:LYS:HG2	1:C:584:VAL:CG1	2.51	0.40
1:B:394:TYR:O	1:B:394:TYR:CG	2.74	0.40
1:E:592:PHE:CD1	1:E:610:LEU:HD22	2.56	0.40
1:C:347:VAL:CG1	1:C:387:ILE:HD13	2.51	0.40
1:C:355:MET:HE1	1:C:391:LEU:O	2.20	0.40
1:C:438:ILE:HD13	1:C:670:PRO:HB3	2.03	0.40
1:C:524:MET:CE	1:C:589:GLN:NE2	2.85	0.40
1:F:153:LEU:HD22	1:F:175:ARG:NH2	2.36	0.40
1:F:551:ILE:CG2	1:F:571:VAL:HG13	2.51	0.40
1:A:433:LEU:HD13	1:A:662:VAL:HG11	2.01	0.40
1:E:521:THR:HB	1:E:626:ILE:HG23	2.03	0.40
1:F:216:ASN:HD22	1:F:216:ASN:N	2.18	0.40
1:A:394:TYR:O	1:A:394:TYR:CG	2.74	0.40
1:B:641:ILE:HD12	1:B:672:MET:HE1	2.03	0.40
1:D:461:ILE:HG23	1:D:462:PRO:HD2	2.03	0.40
1:F:340:GLY:N	1:F:377:MET:O	2.55	0.40
1:C:454:LYS:O	1:C:500:GLN:NE2	2.53	0.40
1:D:487:ILE:HD13	1:D:672:MET:HE2	2.02	0.40
1:D:555:ILE:O	1:D:555:ILE:HG23	2.21	0.40
1:E:347:VAL:CG1	1:E:387:ILE:HD13	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	523/599 (87%)	479 (92%)	40 (8%)	4 (1%)	16	50
1	B	527/599 (88%)	486 (92%)	37 (7%)	4 (1%)	16	50
1	C	527/599 (88%)	493 (94%)	31 (6%)	3 (1%)	21	56
1	D	525/599 (88%)	484 (92%)	37 (7%)	4 (1%)	16	50
1	E	527/599 (88%)	492 (93%)	32 (6%)	3 (1%)	21	56
1	F	528/599 (88%)	498 (94%)	23 (4%)	7 (1%)	9	40
All	All	3157/3594 (88%)	2932 (93%)	200 (6%)	25 (1%)	16	50

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	623	ASN
1	A	398	GLY
1	B	398	GLY
1	C	398	GLY
1	D	398	GLY
1	D	622	GLY
1	E	398	GLY
1	E	483	ASN
1	F	240	LYS
1	F	398	GLY
1	F	483	ASN
1	A	145	GLY
1	E	582	GLU
1	F	439	MET
1	F	561	SER
1	A	483	ASN
1	B	236	LEU
1	C	603	GLU
1	D	603	GLU
1	A	307	PRO
1	B	145	GLY
1	B	603	GLU
1	D	310	PRO
1	F	482	ILE
1	F	310	PRO

5.3.2 Protein sidechains ⓘ

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	358/535 (67%)	335 (94%)	23 (6%)	16	48
1	B	352/535 (66%)	331 (94%)	21 (6%)	17	50
1	C	348/535 (65%)	331 (95%)	17 (5%)	22	55
1	D	340/535 (64%)	321 (94%)	19 (6%)	19	52
1	E	341/535 (64%)	322 (94%)	19 (6%)	19	52
1	F	336/535 (63%)	321 (96%)	15 (4%)	24	58
All	All	2075/3210 (65%)	1961 (94%)	114 (6%)	19	52

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	SER
1	A	150	THR
1	A	153	LEU
1	A	177	ILE
1	A	193	SER
1	A	195	ILE
1	A	211	LYS
1	A	216	ASN
1	A	217	ASP
1	A	273	THR
1	A	274	ILE
1	A	294	SER
1	A	306	VAL
1	A	308	PHE
1	A	322	THR
1	A	356	HIS
1	A	402	LEU
1	A	434	THR
1	A	461	ILE
1	A	507	VAL
1	A	542	THR
1	A	564	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	572	THR
1	B	135	PHE
1	B	150	THR
1	B	177	ILE
1	B	193	SER
1	B	195	ILE
1	B	216	ASN
1	B	273	THR
1	B	274	ILE
1	B	294	SER
1	B	308	PHE
1	B	322	THR
1	B	344	THR
1	B	356	HIS
1	B	377	MET
1	B	447	ASN
1	B	461	ILE
1	B	507	VAL
1	B	553	ILE
1	B	564	ILE
1	B	572	THR
1	B	588	ARG
1	C	177	ILE
1	C	193	SER
1	C	195	ILE
1	C	216	ASN
1	C	273	THR
1	C	274	ILE
1	C	294	SER
1	C	308	PHE
1	C	322	THR
1	C	356	HIS
1	C	461	ILE
1	C	479	THR
1	C	499	THR
1	C	507	VAL
1	C	564	ILE
1	C	572	THR
1	C	615	GLN
1	D	150	THR
1	D	177	ILE
1	D	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	193	SER
1	D	195	ILE
1	D	216	ASN
1	D	273	THR
1	D	274	ILE
1	D	294	SER
1	D	308	PHE
1	D	356	HIS
1	D	461	ILE
1	D	467	ARG
1	D	507	VAL
1	D	564	ILE
1	D	572	THR
1	D	588	ARG
1	D	623	ASN
1	D	626	ILE
1	E	177	ILE
1	E	193	SER
1	E	195	ILE
1	E	216	ASN
1	E	273	THR
1	E	274	ILE
1	E	294	SER
1	E	308	PHE
1	E	356	HIS
1	E	434	THR
1	E	438	ILE
1	E	458	ILE
1	E	460	ILE
1	E	461	ILE
1	E	467	ARG
1	E	479	THR
1	E	564	ILE
1	E	572	THR
1	E	686	VAL
1	F	153	LEU
1	F	177	ILE
1	F	193	SER
1	F	195	ILE
1	F	273	THR
1	F	274	ILE
1	F	294	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	308	PHE
1	F	356	HIS
1	F	434	THR
1	F	461	ILE
1	F	514	ILE
1	F	542	THR
1	F	564	ILE
1	F	572	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	216	ASN
1	A	451	ASN
1	A	538	GLN
1	A	618	GLN
1	A	660	GLN
1	A	678	GLN
1	B	146	HIS
1	B	155	ASN
1	B	216	ASN
1	B	447	ASN
1	B	538	GLN
1	B	624	HIS
1	C	146	HIS
1	C	155	ASN
1	C	180	GLN
1	C	216	ASN
1	C	324	ASN
1	C	376	GLN
1	C	383	GLN
1	C	538	GLN
1	C	615	GLN
1	C	624	HIS
1	C	678	GLN
1	D	146	HIS
1	D	155	ASN
1	D	167	ASN
1	D	216	ASN
1	D	327	HIS
1	D	379	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	538	GLN
1	D	589	GLN
1	D	593	HIS
1	D	618	GLN
1	D	620	GLN
1	D	623	ASN
1	D	624	HIS
1	E	146	HIS
1	E	155	ASN
1	E	216	ASN
1	E	235	ASN
1	E	324	ASN
1	E	376	GLN
1	E	379	GLN
1	E	492	GLN
1	E	505	HIS
1	E	538	GLN
1	E	624	HIS
1	F	155	ASN
1	F	216	ASN
1	F	376	GLN
1	F	435	ASN
1	F	538	GLN
1	F	620	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	537/599 (89%)	0.28	15 (2%)	55	35	57, 63, 66, 69	0
1	B	541/599 (90%)	0.33	20 (3%)	45	28	57, 63, 66, 69	0
1	C	541/599 (90%)	0.40	21 (3%)	43	27	57, 63, 66, 69	0
1	D	539/599 (89%)	0.50	24 (4%)	38	24	57, 63, 66, 69	0
1	E	541/599 (90%)	0.37	17 (3%)	51	32	57, 63, 66, 69	0
1	F	542/599 (90%)	0.43	20 (3%)	45	28	57, 63, 66, 69	0
All	All	3241/3594 (90%)	0.38	117 (3%)	46	28	57, 63, 66, 69	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	200	GLU	4.7
1	D	133	LYS	4.6
1	F	581	GLY	4.5
1	A	581	GLY	4.5
1	D	362	ASP	4.1
1	D	328	ALA	4.0
1	F	406	SER	3.7
1	F	132	CYS	3.5
1	A	404	VAL	3.5
1	F	404	VAL	3.5
1	C	271	ASP	3.4
1	E	266	CYS	3.3
1	C	581	GLY	3.3
1	D	145	GLY	3.3
1	C	133	LYS	3.3
1	B	271	ASP	3.2
1	C	464	ASP	3.2
1	A	574	ASN	3.1
1	D	404	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	200	GLU	3.1
1	D	622	GLY	3.0
1	C	303	ASP	2.9
1	C	402	LEU	2.9
1	B	621	THR	2.9
1	D	574	ASN	2.9
1	E	561	SER	2.8
1	B	428	GLU	2.8
1	D	356	HIS	2.8
1	B	186	CYS	2.7
1	A	188	ASP	2.7
1	A	403	ASP	2.7
1	C	172	ASP	2.7
1	F	438	ILE	2.7
1	B	439	MET	2.7
1	F	336	SER	2.6
1	D	303	ASP	2.6
1	D	509	ASP	2.6
1	B	531	ARG	2.6
1	F	129	ALA	2.6
1	D	464	ASP	2.6
1	D	405	SER	2.6
1	A	115	ILE	2.6
1	E	188	ASP	2.6
1	E	401	GLU	2.6
1	F	405	SER	2.5
1	A	200	GLU	2.5
1	D	559	THR	2.5
1	B	402	LEU	2.5
1	D	134	GLN	2.5
1	E	389	GLN	2.5
1	C	200	GLU	2.5
1	E	464	ASP	2.5
1	A	402	LEU	2.5
1	B	150	THR	2.4
1	C	148	GLN	2.4
1	D	439	MET	2.4
1	F	464	ASP	2.4
1	E	531	ARG	2.4
1	E	543	GLU	2.4
1	D	188	ASP	2.4
1	B	429	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	264	GLU	2.4
1	C	128	SER	2.4
1	C	362	ASP	2.3
1	F	621	THR	2.3
1	C	266	CYS	2.3
1	F	443	MET	2.3
1	D	271	ASP	2.3
1	E	562	GLU	2.3
1	A	290	PRO	2.3
1	D	406	SER	2.3
1	F	399	ASP	2.3
1	B	379	GLN	2.3
1	D	545	SER	2.3
1	D	120	LEU	2.3
1	B	362	ASP	2.3
1	E	622	GLY	2.3
1	E	111	LYS	2.3
1	E	469	ILE	2.2
1	D	308	PHE	2.2
1	C	574	ASN	2.2
1	C	494	ASP	2.2
1	F	691	ASP	2.2
1	F	451	ASN	2.2
1	B	534	ASP	2.2
1	C	196	ASP	2.2
1	E	265	ASP	2.2
1	F	144	SER	2.2
1	F	227	SER	2.2
1	B	425	GLY	2.2
1	B	581	GLY	2.2
1	C	288	LYS	2.2
1	E	581	GLY	2.2
1	A	534	ASP	2.2
1	A	136	ARG	2.1
1	F	674	GLN	2.1
1	A	281	PRO	2.1
1	E	264	GLU	2.1
1	C	404	VAL	2.1
1	C	672	MET	2.1
1	B	133	LYS	2.1
1	B	303	ASP	2.1
1	E	132	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	581	GLY	2.1
1	B	405	SER	2.1
1	C	227	SER	2.1
1	C	509	ASP	2.1
1	F	534	ASP	2.1
1	A	186	CYS	2.1
1	B	533	GLN	2.1
1	A	652	ALA	2.0
1	B	265	ASP	2.0
1	C	308	PHE	2.0
1	B	308	PHE	2.0
1	A	288	LYS	2.0
1	E	436	VAL	2.0
1	F	437	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	1694	1/1	0.95	0.10	82,82,82,82	0
2	CL	F	1692	1/1	0.96	0.09	68,68,68,68	0
2	CL	A	1692	1/1	0.97	0.09	65,65,65,65	0
2	CL	D	1692	1/1	0.97	0.10	78,78,78,78	0
2	CL	E	1692	1/1	0.97	0.12	66,66,66,66	0
2	CL	B	1693	1/1	0.97	0.10	74,74,74,74	0
2	CL	D	1693	1/1	0.98	0.06	40,40,40,40	0
2	CL	C	1692	1/1	0.98	0.05	43,43,43,43	0
2	CL	B	1692	1/1	0.98	0.05	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	E	1693	1/1	0.99	0.05	40,40,40,40	0
2	CL	A	1693	1/1	0.99	0.05	51,51,51,51	0
2	CL	F	1693	1/1	0.99	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.