



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:18 AM UTC

PDB ID : 3IDE / pdb_00003ide
Title : Structure of IPNV subviral particle
Authors : Coulibaly, F.; Chevalier, C.; Delmas, B.; Rey, F.A.
Deposited on : 2009-07-21
Resolution : 3.35 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
Xtrriage (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

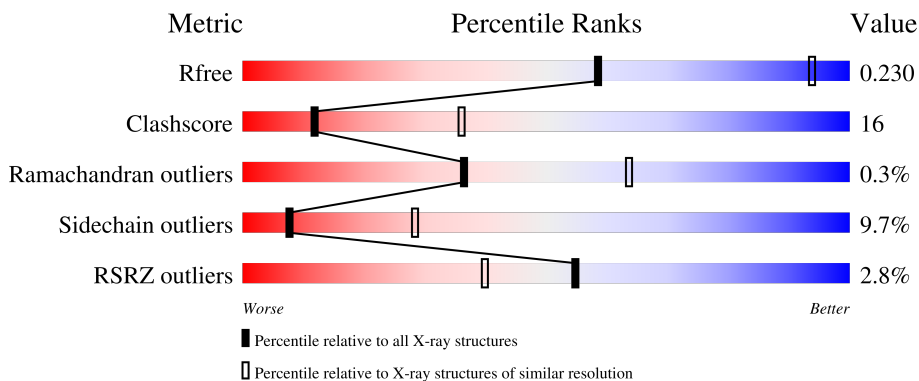
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	442	 3% 59% 30% 5% 6%
1	B	442	 3% 61% 29% 5% 6%
1	C	442	 2% 60% 30% 5% 6%
1	D	442	 4% 60% 30% 5% 6%
1	E	442	 % 59% 30% 5% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16072 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 Capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3208	2013	543	640	12	0	0	0
1	B	416	3216	2019	544	641	12	0	0	0
1	C	415	3208	2013	543	640	12	0	0	0
1	D	416	3216	2019	544	641	12	0	0	0
1	E	415	3208	2013	543	640	12	0	0	0

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Co 1	0	0
2	C	1	Total 1	Co 1	0	0
2	E	1	Total 1	Co 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

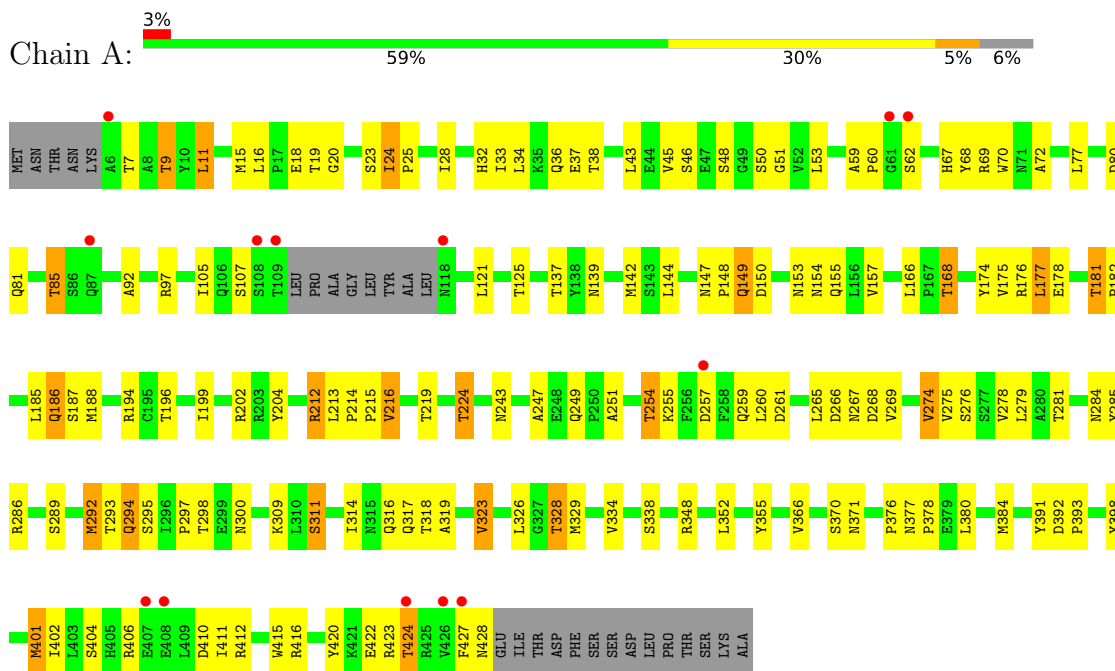
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0
4	E	2	Total O 2 2	0	0

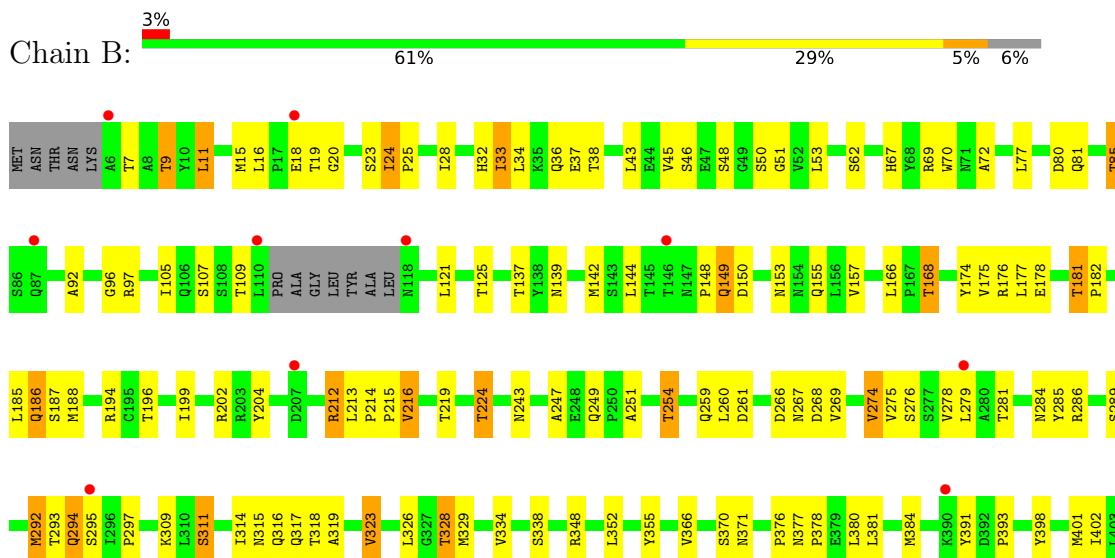
3 Residue-property plots [i](#)

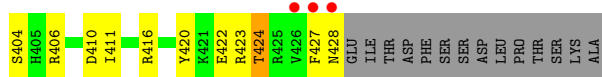
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Capsid protein VP2

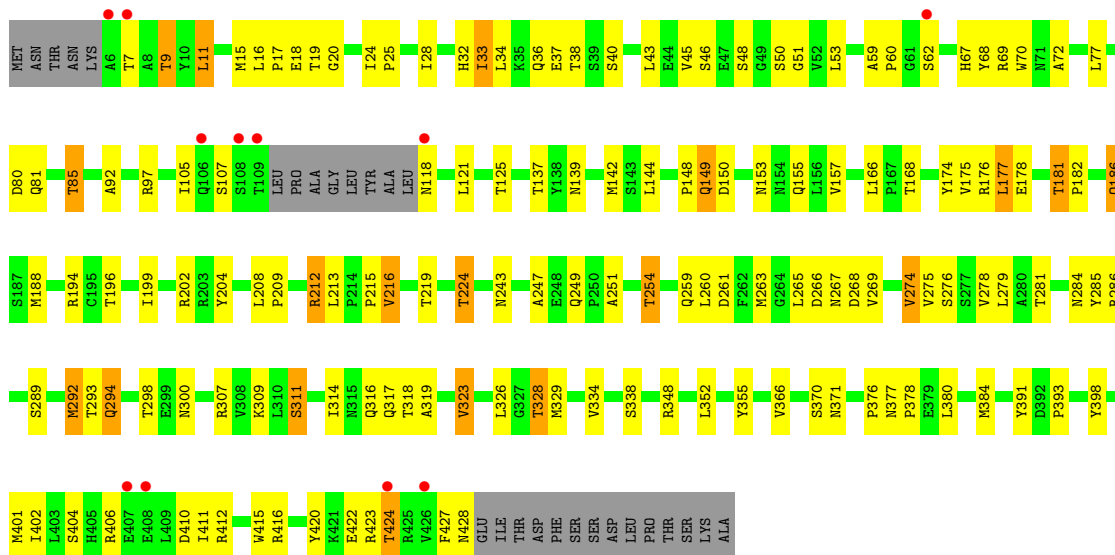


- Molecule 1: Capsid protein VP2

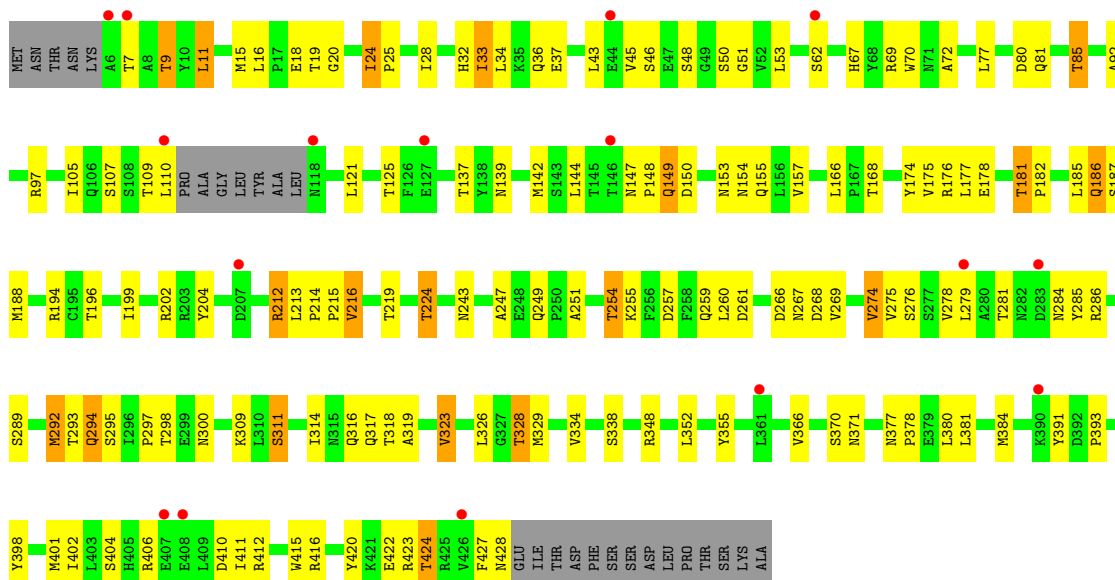




• Molecule 1: Capsid protein VP2

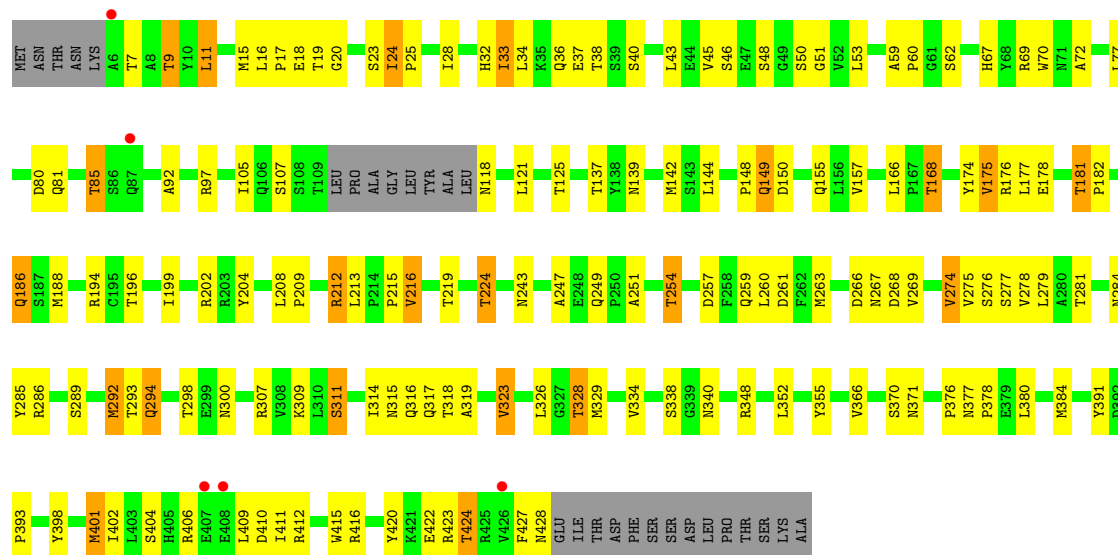


• Molecule 1: Capsid protein VP2



• Molecule 1: Capsid protein VP2





4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	303.43Å 303.43Å 303.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.35 29.75 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.75-3.35) 98.4 (29.75-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.233 0.213 , 0.230	Depositor DCC
R_{free} test set	1992 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	88.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16072	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/3268	0.81	7/4449 (0.2%)
1	B	0.37	0/3276	0.81	7/4460 (0.2%)
1	C	0.39	0/3268	0.81	5/4449 (0.1%)
1	D	0.36	0/3276	0.81	6/4460 (0.1%)
1	E	0.41	0/3268	0.82	6/4449 (0.1%)
All	All	0.38	0/16356	0.81	31/22267 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	HIS	N-CA-C	6.81	117.03	108.45
1	B	32	HIS	N-CA-C	6.58	116.73	108.45
1	E	32	HIS	N-CA-C	6.54	116.69	108.45
1	A	32	HIS	N-CA-C	6.44	116.56	108.45
1	C	32	HIS	N-CA-C	6.20	116.26	108.45
1	D	328	THR	N-CA-C	6.12	118.45	111.11
1	A	20	GLY	CA-C-N	6.01	126.51	120.14
1	A	20	GLY	C-N-CA	6.01	126.51	120.14
1	C	328	THR	N-CA-C	6.01	118.32	111.11
1	A	328	THR	N-CA-C	5.96	118.26	111.11
1	E	328	THR	N-CA-C	5.80	118.07	111.11
1	E	20	GLY	CA-C-N	5.70	126.18	120.14
1	E	20	GLY	C-N-CA	5.70	126.18	120.14
1	B	20	GLY	CA-C-N	5.67	126.15	120.14
1	B	20	GLY	C-N-CA	5.67	126.15	120.14
1	D	20	GLY	CA-C-N	5.58	126.06	120.14
1	D	20	GLY	C-N-CA	5.58	126.06	120.14
1	C	20	GLY	CA-C-N	5.56	126.03	120.14
1	C	20	GLY	C-N-CA	5.56	126.03	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	THR	N-CA-C	5.48	117.69	111.11
1	C	177	LEU	N-CA-C	-5.34	103.47	110.53
1	D	24	ILE	CA-C-N	5.32	126.49	119.84
1	D	24	ILE	C-N-CA	5.32	126.49	119.84
1	A	24	ILE	CA-C-N	5.25	126.40	119.84
1	A	24	ILE	C-N-CA	5.25	126.40	119.84
1	B	96	GLY	N-CA-C	5.17	118.83	110.87
1	E	24	ILE	CA-C-N	5.12	126.24	119.84
1	E	24	ILE	C-N-CA	5.12	126.24	119.84
1	A	177	LEU	N-CA-C	-5.11	103.78	110.53
1	B	24	ILE	CA-C-N	5.01	126.10	119.84
1	B	24	ILE	C-N-CA	5.01	126.10	119.84

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	3208	0	3188	103	0
1	B	3216	0	3199	101	0
1	C	3208	0	3188	104	0
1	D	3216	0	3199	103	0
1	E	3208	0	3188	103	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	16072	0	15962	505	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 16.

All (505) 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:410:ASP:HB3	1:E:423:ARG:HH22	1.18	1.07
1:B:410:ASP:HB3	1:B:423:ARG:HH22	1.17	1.07
1:A:410:ASP:HB3	1:A:423:ARG:HH22	1.17	1.05
1:D:410:ASP:HB3	1:D:423:ARG:HH22	1.17	1.05
1:C:410:ASP:HB3	1:C:423:ARG:HH22	1.17	1.01
1:C:410:ASP:HB3	1:C:423:ARG:NH2	1.90	0.87
1:A:410:ASP:HB3	1:A:423:ARG:NH2	1.90	0.87
1:D:410:ASP:HB3	1:D:423:ARG:NH2	1.89	0.86
1:B:410:ASP:HB3	1:B:423:ARG:NH2	1.90	0.85
1:E:181:THR:HG22	1:E:182:PRO:HD2	1.57	0.84
1:E:410:ASP:HB3	1:E:423:ARG:NH2	1.91	0.84
1:C:181:THR:HG22	1:C:182:PRO:HD2	1.58	0.84
1:D:410:ASP:CB	1:D:423:ARG:HH22	1.93	0.82
1:C:410:ASP:CB	1:C:423:ARG:HH22	1.93	0.82
1:A:391:TYR:CZ	1:A:393:PRO:HG3	2.14	0.82
1:B:391:TYR:CZ	1:B:393:PRO:HG3	2.15	0.81
1:C:391:TYR:CZ	1:C:393:PRO:HG3	2.15	0.81
1:A:181:THR:HG22	1:A:182:PRO:HD2	1.63	0.81
1:D:181:THR:HG22	1:D:182:PRO:HD2	1.62	0.81
1:B:181:THR:HG22	1:B:182:PRO:HD2	1.63	0.80
1:B:410:ASP:CB	1:B:423:ARG:HH22	1.94	0.80
1:E:391:TYR:CZ	1:E:393:PRO:HG3	2.16	0.80
1:E:410:ASP:CB	1:E:423:ARG:HH22	1.94	0.80
1:D:391:TYR:CZ	1:D:393:PRO:HG3	2.17	0.79
1:A:410:ASP:CB	1:A:423:ARG:HH22	1.93	0.78
1:B:292:MET:HE2	1:B:294:GLN:OE1	1.84	0.77
1:A:292:MET:HE2	1:A:294:GLN:OE1	1.84	0.76
1:D:292:MET:HE2	1:D:294:GLN:OE1	1.85	0.75
1:E:292:MET:HE2	1:E:294:GLN:OE1	1.89	0.73
1:C:292:MET:HE2	1:C:294:GLN:OE1	1.88	0.72
1:E:259:GLN:HG2	1:E:275:VAL:HG22	1.73	0.71
1:B:254:THR:HG21	1:B:319:ALA:HB2	1.72	0.71
1:B:259:GLN:HG2	1:B:275:VAL:HG22	1.72	0.70
1:D:259:GLN:HG2	1:D:275:VAL:HG22	1.72	0.70
1:E:212:ARG:NH1	1:E:215:PRO:HG3	2.06	0.70
1:C:274:VAL:HG21	1:C:294:GLN:HG3	1.74	0.70
1:A:259:GLN:HG2	1:A:275:VAL:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLN:HG2	1:C:275:VAL:HG22	1.73	0.70
1:A:254:THR:HG21	1:A:319:ALA:HB2	1.73	0.69
1:E:254:THR:HG21	1:E:319:ALA:HB2	1.72	0.69
1:C:254:THR:HG21	1:C:319:ALA:HB2	1.73	0.69
1:C:150:ASP:CG	1:C:406:ARG:HH22	2.01	0.69
1:B:150:ASP:CG	1:B:406:ARG:HH22	2.01	0.69
1:B:212:ARG:NH1	1:B:215:PRO:HG3	2.08	0.69
1:D:254:THR:HG21	1:D:319:ALA:HB2	1.73	0.69
1:C:212:ARG:NH1	1:C:215:PRO:HG3	2.08	0.68
1:A:50:SER:HB3	1:A:70:TRP:CD1	2.28	0.68
1:A:274:VAL:HG21	1:A:294:GLN:HG3	1.75	0.68
1:C:50:SER:HB3	1:C:70:TRP:CD1	2.28	0.68
1:D:150:ASP:CG	1:D:406:ARG:HH22	2.01	0.68
1:D:274:VAL:HG21	1:D:294:GLN:HG3	1.76	0.68
1:E:50:SER:HB3	1:E:70:TRP:CD1	2.28	0.68
1:A:212:ARG:NH1	1:A:215:PRO:HG3	2.09	0.68
1:C:38:THR:HB	1:D:153:ASN:ND2	2.10	0.67
1:D:178:GLU:HG2	1:D:196:THR:HA	1.76	0.67
1:A:150:ASP:CG	1:A:406:ARG:HH22	2.02	0.67
1:C:40:SER:HB3	1:D:154:ASN:ND2	2.10	0.67
1:E:150:ASP:CG	1:E:406:ARG:HH22	2.01	0.67
1:B:178:GLU:HG2	1:B:196:THR:HA	1.77	0.67
1:B:274:VAL:HG21	1:B:294:GLN:HG3	1.76	0.67
1:D:212:ARG:NH1	1:D:215:PRO:HG3	2.10	0.67
1:E:178:GLU:HG2	1:E:196:THR:HA	1.77	0.67
1:B:50:SER:HB3	1:B:70:TRP:CD1	2.30	0.67
1:A:178:GLU:HG2	1:A:196:THR:HA	1.77	0.66
1:E:274:VAL:HG21	1:E:294:GLN:HG3	1.76	0.66
1:D:50:SER:HB3	1:D:70:TRP:CD1	2.31	0.66
1:C:380:LEU:HD13	1:C:384:MET:HE1	1.78	0.66
1:C:178:GLU:HG2	1:C:196:THR:HA	1.77	0.65
1:A:380:LEU:HD13	1:A:384:MET:HE1	1.78	0.65
1:E:212:ARG:HH12	1:E:215:PRO:HG3	1.63	0.64
1:E:380:LEU:HD13	1:E:384:MET:HE1	1.79	0.64
1:D:109:THR:HG23	1:E:118:ASN:ND2	2.12	0.64
1:D:380:LEU:HD13	1:D:384:MET:HE1	1.80	0.64
1:D:420:TYR:O	1:D:424:THR:HB	1.99	0.63
1:A:212:ARG:HH12	1:A:215:PRO:HG3	1.64	0.62
1:C:212:ARG:HH12	1:C:215:PRO:HG3	1.64	0.62
1:E:420:TYR:O	1:E:424:THR:HB	2.00	0.62
1:B:212:ARG:HH12	1:B:215:PRO:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:HD13	1:B:384:MET:HE1	1.80	0.62
1:C:420:TYR:O	1:C:424:THR:HB	2.00	0.61
1:B:97:ARG:HD2	1:B:174:TYR:CE1	2.35	0.61
1:A:420:TYR:O	1:A:424:THR:HB	2.00	0.61
1:B:420:TYR:O	1:B:424:THR:HB	2.00	0.61
1:C:97:ARG:HD2	1:C:174:TYR:CE1	2.36	0.61
1:D:243:ASN:CG	1:D:329:MET:HB2	2.26	0.61
1:D:212:ARG:HH12	1:D:215:PRO:HG3	1.65	0.60
1:D:401:MET:O	1:D:404:SER:HB3	2.01	0.60
1:A:243:ASN:CG	1:A:329:MET:HB2	2.27	0.60
1:D:286:ARG:HE	1:D:286:ARG:HA	1.67	0.60
1:E:148:PRO:HG2	1:E:149:GLN:NE2	2.17	0.59
1:B:53:LEU:HD21	1:B:366:VAL:HG21	1.85	0.59
1:E:286:ARG:HA	1:E:286:ARG:HE	1.67	0.59
1:C:243:ASN:CG	1:C:329:MET:HB2	2.27	0.59
1:C:286:ARG:HE	1:C:286:ARG:HA	1.67	0.59
1:D:97:ARG:HD2	1:D:174:TYR:CE1	2.37	0.59
1:D:216:VAL:HG21	1:D:314:ILE:HD11	1.85	0.59
1:E:53:LEU:HD21	1:E:366:VAL:HG21	1.85	0.59
1:B:401:MET:O	1:B:404:SER:HB3	2.03	0.59
1:C:148:PRO:HG2	1:C:149:GLN:NE2	2.18	0.59
1:C:401:MET:O	1:C:404:SER:HB3	2.03	0.59
1:A:53:LEU:HD21	1:A:366:VAL:HG21	1.85	0.58
1:B:286:ARG:HE	1:B:286:ARG:HA	1.67	0.58
1:D:53:LEU:HD21	1:D:366:VAL:HG21	1.86	0.58
1:B:243:ASN:CG	1:B:329:MET:HB2	2.27	0.58
1:A:97:ARG:HD2	1:A:174:TYR:CE1	2.39	0.58
1:B:216:VAL:HG21	1:B:314:ILE:HD11	1.85	0.58
1:A:401:MET:O	1:A:404:SER:HB3	2.04	0.58
1:E:97:ARG:HD2	1:E:174:TYR:CE1	2.37	0.58
1:E:401:MET:O	1:E:404:SER:HB3	2.02	0.58
1:A:216:VAL:HG21	1:A:314:ILE:HD11	1.86	0.58
1:A:286:ARG:HE	1:A:286:ARG:HA	1.68	0.58
1:D:148:PRO:HG2	1:D:149:GLN:NE2	2.19	0.57
1:C:53:LEU:HD21	1:C:366:VAL:HG21	1.86	0.57
1:A:148:PRO:HG2	1:A:149:GLN:NE2	2.20	0.56
1:C:144:LEU:HD11	1:C:352:LEU:HD12	1.88	0.56
1:E:51:GLY:HA3	1:E:355:TYR:CZ	2.40	0.56
1:E:216:VAL:HG21	1:E:314:ILE:HD11	1.87	0.56
1:A:153:ASN:ND2	1:E:38:THR:HB	2.21	0.56
1:C:377:ASN:HB2	1:C:378:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:ASN:CG	1:E:329:MET:HB2	2.31	0.56
1:B:148:PRO:HG2	1:B:149:GLN:NE2	2.20	0.55
1:E:144:LEU:HD11	1:E:352:LEU:HD12	1.88	0.55
1:D:109:THR:O	1:D:110:LEU:HD23	2.06	0.55
1:C:51:GLY:HA3	1:C:355:TYR:CZ	2.42	0.55
1:A:144:LEU:HD11	1:A:352:LEU:HD12	1.89	0.55
1:B:144:LEU:HD11	1:B:352:LEU:HD12	1.89	0.55
1:A:51:GLY:HA3	1:A:355:TYR:CZ	2.42	0.54
1:C:216:VAL:HG21	1:C:314:ILE:HD11	1.88	0.54
1:A:377:ASN:HB2	1:A:378:PRO:HD2	1.89	0.54
1:C:48:SER:HB3	1:C:72:ALA:HA	1.90	0.54
1:D:377:ASN:HB2	1:D:378:PRO:HD2	1.88	0.54
1:E:48:SER:HB3	1:E:72:ALA:HA	1.90	0.54
1:B:51:GLY:HA3	1:B:355:TYR:CZ	2.43	0.54
1:D:380:LEU:HD22	1:D:384:MET:HE2	1.90	0.54
1:D:53:LEU:HD23	1:D:105:ILE:HD13	1.90	0.54
1:B:377:ASN:HB2	1:B:378:PRO:HD2	1.90	0.53
1:B:48:SER:HB3	1:B:72:ALA:HA	1.90	0.53
1:B:53:LEU:HD23	1:B:105:ILE:HD13	1.90	0.53
1:D:48:SER:HB3	1:D:72:ALA:HA	1.90	0.53
1:D:144:LEU:HD11	1:D:352:LEU:HD12	1.89	0.53
1:E:377:ASN:HB2	1:E:378:PRO:HD2	1.89	0.53
1:A:48:SER:HB3	1:A:72:ALA:HA	1.89	0.53
1:E:276:SER:CB	1:E:292:MET:HE3	2.39	0.53
1:D:51:GLY:HA3	1:D:355:TYR:CZ	2.44	0.53
1:E:11:LEU:HD11	1:E:402:ILE:HG13	1.91	0.53
1:E:181:THR:CG2	1:E:182:PRO:HD2	2.33	0.52
1:B:380:LEU:HD22	1:B:384:MET:HE2	1.92	0.52
1:B:249:GLN:HG2	1:B:285:TYR:CE1	2.45	0.52
1:D:70:TRP:CE2	1:D:77:LEU:HD21	2.45	0.52
1:E:53:LEU:HD23	1:E:105:ILE:HD13	1.92	0.52
1:C:11:LEU:HD11	1:C:402:ILE:HG13	1.91	0.52
1:A:53:LEU:HD23	1:A:105:ILE:HD13	1.91	0.52
1:C:181:THR:CG2	1:C:182:PRO:HD2	2.34	0.52
1:A:70:TRP:CE2	1:A:77:LEU:HD21	2.45	0.52
1:A:107:SER:HB3	1:A:157:VAL:HG12	1.91	0.52
1:B:276:SER:CB	1:B:292:MET:HE3	2.40	0.51
1:B:107:SER:HB3	1:B:157:VAL:HG12	1.92	0.51
1:B:202:ARG:HD3	1:B:204:TYR:CE1	2.45	0.51
1:A:121:LEU:HG	1:A:157:VAL:HG22	1.93	0.51
1:C:266:ASP:N	1:C:266:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD11	1:B:402:ILE:HG13	1.93	0.51
1:B:70:TRP:CE2	1:B:77:LEU:HD21	2.45	0.51
1:E:80:ASP:OD1	1:E:81:GLN:HG2	2.11	0.51
1:A:137:THR:HG22	1:A:139:ASN:H	1.76	0.51
1:C:276:SER:CB	1:C:292:MET:HE3	2.40	0.51
1:E:286:ARG:HA	1:E:286:ARG:NE	2.26	0.51
1:A:186:GLN:CD	1:A:186:GLN:H	2.19	0.51
1:C:202:ARG:HD3	1:C:204:TYR:CE1	2.46	0.51
1:A:249:GLN:HG2	1:A:285:TYR:CE1	2.46	0.51
1:C:70:TRP:CE2	1:C:77:LEU:HD21	2.46	0.51
1:D:144:LEU:CD1	1:D:352:LEU:HD12	2.41	0.51
1:C:186:GLN:CD	1:C:186:GLN:H	2.19	0.50
1:D:266:ASP:OD1	1:D:266:ASP:N	2.44	0.50
1:B:176:ARG:HG3	1:B:177:LEU:O	2.11	0.50
1:C:121:LEU:HG	1:C:157:VAL:HG22	1.93	0.50
1:C:137:THR:HG22	1:C:139:ASN:H	1.76	0.50
1:E:137:THR:HG22	1:E:139:ASN:H	1.77	0.50
1:A:406:ARG:O	1:A:406:ARG:HG2	2.12	0.50
1:B:213:LEU:HD21	1:B:326:LEU:HD21	1.93	0.50
1:B:406:ARG:O	1:B:406:ARG:HG2	2.10	0.50
1:B:137:THR:HG22	1:B:139:ASN:H	1.77	0.50
1:C:53:LEU:HD23	1:C:105:ILE:HD13	1.93	0.50
1:D:276:SER:CB	1:D:292:MET:HE3	2.41	0.50
1:E:249:GLN:HG2	1:E:285:TYR:CE1	2.46	0.50
1:A:181:THR:CG2	1:A:182:PRO:HD2	2.38	0.50
1:A:276:SER:CB	1:A:292:MET:HE3	2.42	0.50
1:B:286:ARG:HA	1:B:286:ARG:NE	2.26	0.50
1:D:11:LEU:HD11	1:D:402:ILE:HG13	1.92	0.50
1:B:150:ASP:OD1	1:B:406:ARG:NH2	2.43	0.50
1:D:202:ARG:HD3	1:D:204:TYR:CE1	2.47	0.50
1:C:249:GLN:HG2	1:C:285:TYR:CE1	2.47	0.50
1:B:109:THR:HG23	1:C:118:ASN:ND2	2.27	0.49
1:C:107:SER:HB3	1:C:157:VAL:HG12	1.93	0.49
1:D:249:GLN:HG2	1:D:285:TYR:CE1	2.47	0.49
1:C:176:ARG:HG3	1:C:177:LEU:O	2.12	0.49
1:E:202:ARG:HD3	1:E:204:TYR:CE1	2.47	0.49
1:E:276:SER:HB3	1:E:292:MET:HE3	1.93	0.49
1:A:11:LEU:HD11	1:A:402:ILE:HG13	1.94	0.49
1:A:16:LEU:O	1:A:19:THR:HB	2.12	0.49
1:A:144:LEU:CD1	1:A:352:LEU:HD12	2.43	0.49
1:B:274:VAL:HG21	1:B:294:GLN:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:SER:HB3	1:C:292:MET:HE3	1.94	0.49
1:D:107:SER:HB3	1:D:157:VAL:HG12	1.94	0.49
1:D:286:ARG:HA	1:D:286:ARG:NE	2.25	0.49
1:A:46:SER:HB3	1:A:69:ARG:HD3	1.95	0.49
1:B:80:ASP:OD1	1:B:81:GLN:HG2	2.12	0.49
1:B:266:ASP:OD1	1:B:266:ASP:N	2.45	0.49
1:C:274:VAL:HG21	1:C:294:GLN:CG	2.42	0.49
1:D:254:THR:HG22	1:D:316:GLN:HG3	1.94	0.49
1:A:254:THR:HG22	1:A:316:GLN:HG3	1.95	0.49
1:B:121:LEU:HG	1:B:157:VAL:HG22	1.94	0.49
1:C:16:LEU:O	1:C:19:THR:HB	2.13	0.49
1:C:144:LEU:CD1	1:C:352:LEU:HD12	2.42	0.49
1:D:80:ASP:OD1	1:D:81:GLN:HG2	2.13	0.49
1:E:46:SER:HB3	1:E:69:ARG:HD3	1.95	0.49
1:B:144:LEU:CD1	1:B:352:LEU:HD12	2.43	0.49
1:E:406:ARG:O	1:E:406:ARG:HG2	2.11	0.49
1:A:266:ASP:OD1	1:A:266:ASP:N	2.45	0.49
1:E:107:SER:HB3	1:E:157:VAL:HG12	1.95	0.49
1:C:150:ASP:OD1	1:C:406:ARG:NH2	2.45	0.48
1:D:137:THR:HG22	1:D:139:ASN:H	1.77	0.48
1:D:176:ARG:HG3	1:D:177:LEU:O	2.13	0.48
1:D:251:ALA:HB3	1:D:318:THR:HB	1.95	0.48
1:A:38:THR:HB	1:B:153:ASN:ND2	2.29	0.48
1:B:251:ALA:HB3	1:B:318:THR:HB	1.95	0.48
1:A:150:ASP:OD1	1:A:406:ARG:NH2	2.46	0.48
1:A:224:THR:HA	1:A:311:SER:HB3	1.95	0.48
1:B:276:SER:HB3	1:B:292:MET:HE3	1.95	0.48
1:E:121:LEU:HG	1:E:157:VAL:HG22	1.94	0.48
1:A:251:ALA:HB3	1:A:318:THR:HB	1.95	0.48
1:C:80:ASP:OD1	1:C:81:GLN:HG2	2.14	0.48
1:C:254:THR:HG22	1:C:316:GLN:HG3	1.95	0.48
1:D:213:LEU:HD21	1:D:326:LEU:HD21	1.95	0.48
1:E:144:LEU:CD1	1:E:352:LEU:HD12	2.43	0.48
1:A:176:ARG:HG3	1:A:177:LEU:O	2.14	0.48
1:B:254:THR:HG22	1:B:316:GLN:HG3	1.94	0.48
1:C:46:SER:HB3	1:C:69:ARG:HD3	1.95	0.48
1:A:274:VAL:HG21	1:A:294:GLN:CG	2.42	0.48
1:C:251:ALA:HB3	1:C:318:THR:HB	1.95	0.48
1:A:28:ILE:HG22	1:A:28:ILE:O	2.13	0.48
1:C:380:LEU:HD22	1:C:384:MET:HE2	1.94	0.48
1:D:46:SER:HB3	1:D:69:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:THR:HA	1:D:311:SER:HB3	1.96	0.48
1:E:293:THR:O	1:E:293:THR:HG22	2.13	0.48
1:C:406:ARG:O	1:C:406:ARG:HG2	2.14	0.48
1:D:274:VAL:HG21	1:D:294:GLN:CG	2.43	0.48
1:A:80:ASP:OD1	1:A:81:GLN:HG2	2.14	0.47
1:B:16:LEU:O	1:B:19:THR:HB	2.14	0.47
1:B:411:ILE:HD12	1:B:411:ILE:N	2.29	0.47
1:D:121:LEU:HG	1:D:157:VAL:HG22	1.94	0.47
1:E:266:ASP:N	1:E:266:ASP:OD1	2.46	0.47
1:E:380:LEU:HD22	1:E:384:MET:HE2	1.96	0.47
1:A:202:ARG:HD3	1:A:204:TYR:CE1	2.49	0.47
1:B:46:SER:HB3	1:B:69:ARG:HD3	1.96	0.47
1:C:36:GLN:HG3	1:C:371:ASN:OD1	2.14	0.47
1:D:150:ASP:OD1	1:D:406:ARG:NH2	2.45	0.47
1:A:59:ALA:HA	1:A:60:PRO:HD3	1.79	0.47
1:B:105:ILE:HG12	1:B:366:VAL:HG22	1.96	0.47
1:D:181:THR:CG2	1:D:182:PRO:HD2	2.37	0.47
1:A:213:LEU:HD21	1:A:326:LEU:HD21	1.96	0.47
1:C:391:TYR:CE1	1:C:393:PRO:HG3	2.49	0.47
1:B:181:THR:CG2	1:B:182:PRO:HD2	2.38	0.47
1:C:107:SER:HB3	1:C:157:VAL:CG1	2.45	0.47
1:D:16:LEU:O	1:D:19:THR:HB	2.15	0.47
1:C:213:LEU:HD21	1:C:326:LEU:HD21	1.96	0.47
1:E:16:LEU:O	1:E:19:THR:HB	2.14	0.47
1:E:150:ASP:OD1	1:E:406:ARG:NH2	2.44	0.47
1:C:293:THR:HG22	1:C:293:THR:O	2.13	0.47
1:C:59:ALA:HA	1:C:60:PRO:HD3	1.79	0.47
1:B:224:THR:HA	1:B:311:SER:HB3	1.96	0.47
1:B:286:ARG:O	1:B:328:THR:HG21	2.15	0.47
1:E:36:GLN:HG3	1:E:371:ASN:OD1	2.15	0.47
1:E:176:ARG:HG3	1:E:177:LEU:O	2.15	0.47
1:E:254:THR:HG22	1:E:316:GLN:HG3	1.96	0.47
1:A:286:ARG:HA	1:A:286:ARG:NE	2.26	0.47
1:D:380:LEU:HD22	1:D:384:MET:CE	2.45	0.47
1:C:411:ILE:N	1:C:411:ILE:HD12	2.31	0.46
1:C:427:PHE:O	1:C:428:ASN:HB2	2.15	0.46
1:B:186:GLN:H	1:B:186:GLN:CD	2.19	0.46
1:D:276:SER:HB3	1:D:292:MET:HE3	1.96	0.46
1:D:427:PHE:O	1:D:428:ASN:HB2	2.16	0.46
1:A:15:MET:HE1	1:A:411:ILE:CG2	2.45	0.46
1:A:43:LEU:HD13	1:A:67:HIS:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:SER:HB3	1:A:157:VAL:CG1	2.45	0.46
1:B:427:PHE:O	1:B:428:ASN:HB2	2.16	0.46
1:D:216:VAL:HG21	1:D:314:ILE:CD1	2.45	0.46
1:E:186:GLN:H	1:E:186:GLN:CD	2.19	0.46
1:E:251:ALA:HB3	1:E:318:THR:HB	1.96	0.46
1:D:406:ARG:O	1:D:406:ARG:HG2	2.14	0.46
1:A:11:LEU:HD12	1:A:398:TYR:CE2	2.51	0.46
1:A:36:GLN:HG3	1:A:371:ASN:OD1	2.16	0.46
1:A:45:VAL:HG13	1:A:355:TYR:HE1	1.81	0.46
1:B:107:SER:HB3	1:B:157:VAL:CG1	2.45	0.46
1:B:216:VAL:HG21	1:B:314:ILE:CD1	2.45	0.46
1:E:224:THR:HA	1:E:311:SER:HB3	1.96	0.46
1:E:427:PHE:O	1:E:428:ASN:HB2	2.15	0.46
1:A:391:TYR:CE1	1:A:393:PRO:HG3	2.50	0.46
1:B:380:LEU:HD22	1:B:384:MET:CE	2.46	0.46
1:C:410:ASP:HB3	1:C:423:ARG:CZ	2.46	0.46
1:D:15:MET:HE1	1:D:411:ILE:CG2	2.46	0.46
1:E:391:TYR:CE1	1:E:393:PRO:HG3	2.51	0.46
1:A:142:MET:HE2	1:A:142:MET:HA	1.97	0.46
1:A:276:SER:HB3	1:A:292:MET:HE3	1.97	0.46
1:B:33:ILE:HD13	1:B:33:ILE:HA	1.77	0.46
1:D:261:ASP:HB2	1:D:309:LYS:HB3	1.98	0.46
1:A:380:LEU:HD22	1:A:384:MET:HE2	1.96	0.46
1:C:15:MET:HE1	1:C:411:ILE:CG2	2.46	0.46
1:E:107:SER:HB3	1:E:157:VAL:CG1	2.46	0.46
1:E:284:ASN:OD1	1:E:284:ASN:C	2.59	0.46
1:A:188:MET:HB3	1:A:188:MET:HE2	1.68	0.45
1:C:224:THR:HA	1:C:311:SER:HB3	1.96	0.45
1:E:33:ILE:HD13	1:E:33:ILE:HA	1.77	0.45
1:E:213:LEU:HD21	1:E:326:LEU:HD21	1.99	0.45
1:B:293:THR:HG22	1:B:293:THR:O	2.15	0.45
1:D:36:GLN:HG3	1:D:371:ASN:OD1	2.16	0.45
1:A:261:ASP:HB2	1:A:309:LYS:HB3	1.98	0.45
1:A:286:ARG:O	1:A:328:THR:HG21	2.15	0.45
1:B:38:THR:HB	1:C:153:ASN:ND2	2.32	0.45
1:B:37:GLU:HB3	1:B:85:THR:CG2	2.46	0.45
1:C:155:GLN:NE2	1:C:416:ARG:HB3	2.31	0.45
1:C:286:ARG:HA	1:C:286:ARG:NE	2.25	0.45
1:D:37:GLU:HB3	1:D:85:THR:CG2	2.46	0.45
1:E:43:LEU:HD13	1:E:67:HIS:CG	2.51	0.45
1:A:105:ILE:HG12	1:A:366:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:HB2	1:B:309:LYS:HB3	1.99	0.45
1:D:107:SER:HB3	1:D:157:VAL:CG1	2.46	0.45
1:D:274:VAL:HG11	1:D:294:GLN:HG3	1.98	0.45
1:E:15:MET:HE1	1:E:411:ILE:CG2	2.47	0.45
1:E:317:GLN:C	1:E:319:ALA:H	2.25	0.45
1:D:293:THR:HG22	1:D:293:THR:O	2.16	0.45
1:C:142:MET:HE2	1:C:142:MET:HA	1.99	0.45
1:D:142:MET:HA	1:D:142:MET:HE2	1.98	0.45
1:D:286:ARG:O	1:D:328:THR:HG21	2.16	0.45
1:E:261:ASP:HB2	1:E:309:LYS:HB3	1.99	0.45
1:A:411:ILE:N	1:A:411:ILE:HD12	2.32	0.45
1:D:43:LEU:HD13	1:D:67:HIS:CG	2.52	0.45
1:B:11:LEU:HD12	1:B:398:TYR:CE2	2.52	0.45
1:D:186:GLN:CD	1:D:186:GLN:H	2.20	0.45
1:D:411:ILE:HD12	1:D:411:ILE:N	2.32	0.45
1:A:216:VAL:HG21	1:A:314:ILE:CD1	2.46	0.45
1:B:36:GLN:HG3	1:B:371:ASN:OD1	2.16	0.45
1:B:166:LEU:HD11	1:B:411:ILE:HG22	1.98	0.45
1:C:286:ARG:O	1:C:328:THR:HG21	2.17	0.45
1:B:43:LEU:HD13	1:B:67:HIS:CG	2.52	0.44
1:B:142:MET:HE2	1:B:142:MET:HA	1.98	0.44
1:B:391:TYR:CE1	1:B:393:PRO:HG3	2.50	0.44
1:C:43:LEU:HD13	1:C:67:HIS:CG	2.51	0.44
1:C:45:VAL:HG13	1:C:355:TYR:HE1	1.82	0.44
1:D:166:LEU:HD11	1:D:411:ILE:HG22	1.99	0.44
1:C:37:GLU:HB3	1:C:85:THR:CG2	2.47	0.44
1:C:423:ARG:HE	1:C:423:ARG:HB3	1.56	0.44
1:E:155:GLN:NE2	1:E:416:ARG:HB3	2.32	0.44
1:A:37:GLU:HB3	1:A:85:THR:CG2	2.48	0.44
1:A:427:PHE:O	1:A:428:ASN:HB2	2.16	0.44
1:B:45:VAL:HG13	1:B:355:TYR:HE1	1.82	0.44
1:E:50:SER:HB3	1:E:70:TRP:HD1	1.80	0.44
1:E:37:GLU:HB3	1:E:85:THR:CG2	2.47	0.44
1:E:45:VAL:HG13	1:E:355:TYR:HE1	1.83	0.44
1:E:260:LEU:HB3	1:E:274:VAL:HG12	2.00	0.44
1:E:411:ILE:N	1:E:411:ILE:HD12	2.32	0.44
1:A:410:ASP:HB3	1:A:423:ARG:CZ	2.45	0.44
1:C:28:ILE:HG22	1:C:28:ILE:O	2.18	0.44
1:C:261:ASP:HB2	1:C:309:LYS:HB3	2.00	0.44
1:C:284:ASN:OD1	1:C:284:ASN:C	2.60	0.44
1:C:380:LEU:HD22	1:C:384:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:THR:C	1:D:9:THR:H	2.26	0.44
1:D:45:VAL:HG13	1:D:355:TYR:HE1	1.83	0.44
1:A:260:LEU:HB3	1:A:274:VAL:HG12	2.00	0.44
1:B:274:VAL:HG11	1:B:294:GLN:HG3	2.00	0.44
1:D:33:ILE:HD13	1:D:33:ILE:HA	1.78	0.44
1:D:410:ASP:HB3	1:D:423:ARG:CZ	2.46	0.44
1:E:11:LEU:HD12	1:E:398:TYR:CE2	2.52	0.44
1:E:105:ILE:HG12	1:E:366:VAL:HG22	2.00	0.44
1:A:154:ASN:ND2	1:E:40:SER:HB3	2.33	0.44
1:E:28:ILE:O	1:E:28:ILE:HG22	2.16	0.44
1:C:7:THR:C	1:C:9:THR:H	2.26	0.44
1:C:105:ILE:HG12	1:C:366:VAL:HG22	2.00	0.44
1:C:317:GLN:C	1:C:319:ALA:H	2.25	0.44
1:E:92:ALA:C	1:E:377:ASN:HD22	2.26	0.44
1:E:166:LEU:HD11	1:E:411:ILE:HG22	2.00	0.44
1:C:50:SER:HB3	1:C:70:TRP:HD1	1.81	0.43
1:C:292:MET:HG3	1:C:334:VAL:HG22	2.00	0.43
1:E:142:MET:HE2	1:E:142:MET:HA	1.99	0.43
1:A:7:THR:C	1:A:9:THR:H	2.26	0.43
1:A:274:VAL:HG11	1:A:294:GLN:HG3	1.99	0.43
1:A:317:GLN:C	1:A:319:ALA:H	2.27	0.43
1:E:286:ARG:O	1:E:328:THR:HG21	2.18	0.43
1:B:15:MET:HE1	1:B:411:ILE:CG2	2.47	0.43
1:C:166:LEU:HD11	1:C:411:ILE:HG22	2.00	0.43
1:A:247:ALA:HB2	1:A:323:VAL:HG23	2.00	0.43
1:C:274:VAL:HG11	1:C:294:GLN:HG3	2.00	0.43
1:B:38:THR:HB	1:C:153:ASN:HD22	1.84	0.43
1:B:317:GLN:C	1:B:319:ALA:H	2.26	0.43
1:E:216:VAL:HG21	1:E:314:ILE:CD1	2.47	0.43
1:E:380:LEU:HB3	1:E:384:MET:HE2	2.01	0.43
1:A:293:THR:HG22	1:A:293:THR:O	2.18	0.43
1:B:188:MET:HE2	1:B:188:MET:HB3	1.71	0.43
1:C:260:LEU:HB3	1:C:274:VAL:HG12	2.01	0.43
1:D:105:ILE:HG12	1:D:366:VAL:HG22	2.01	0.43
1:E:59:ALA:HA	1:E:60:PRO:HD3	1.79	0.43
1:E:274:VAL:HG21	1:E:294:GLN:CG	2.44	0.43
1:E:412:ARG:HB2	1:E:415:TRP:CE2	2.53	0.43
1:A:166:LEU:HD11	1:A:411:ILE:HG22	2.00	0.43
1:A:168:THR:O	1:A:168:THR:OG1	2.36	0.43
1:B:50:SER:HB3	1:B:70:TRP:HD1	1.82	0.43
1:A:380:LEU:HD22	1:A:384:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ALA:C	1:B:377:ASN:HD22	2.26	0.43
1:C:188:MET:HB3	1:C:188:MET:HE2	1.68	0.43
1:C:380:LEU:HB3	1:C:384:MET:HE2	2.01	0.43
1:C:412:ARG:HB2	1:C:415:TRP:CE2	2.53	0.43
1:B:247:ALA:HB2	1:B:323:VAL:HG23	2.00	0.43
1:D:317:GLN:C	1:D:319:ALA:H	2.26	0.43
1:E:380:LEU:HD22	1:E:384:MET:CE	2.49	0.43
1:C:11:LEU:HD12	1:C:398:TYR:CE2	2.54	0.42
1:D:247:ALA:HB2	1:D:323:VAL:HG23	2.01	0.42
1:E:7:THR:C	1:E:9:THR:H	2.27	0.42
1:A:412:ARG:HB2	1:A:415:TRP:CE2	2.54	0.42
1:E:208:LEU:HA	1:E:209:PRO:HD3	1.82	0.42
1:B:28:ILE:O	1:B:28:ILE:HG22	2.19	0.42
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.80	0.42
1:B:295:SER:O	1:B:297:PRO:HD3	2.19	0.42
1:D:11:LEU:HD12	1:D:398:TYR:CE2	2.54	0.42
1:D:24:ILE:HA	1:D:25:PRO:HD3	1.66	0.42
1:B:7:THR:C	1:B:9:THR:H	2.27	0.42
1:C:24:ILE:HA	1:C:25:PRO:HD3	1.67	0.42
1:A:155:GLN:NE2	1:A:416:ARG:HB3	2.35	0.42
1:B:260:LEU:HB3	1:B:274:VAL:HG12	2.01	0.42
1:B:284:ASN:OD1	1:B:284:ASN:C	2.62	0.42
1:D:284:ASN:OD1	1:D:284:ASN:C	2.62	0.42
1:E:410:ASP:HB3	1:E:423:ARG:CZ	2.47	0.42
1:D:28:ILE:O	1:D:28:ILE:HG22	2.18	0.42
1:D:422:GLU:C	1:D:424:THR:H	2.28	0.42
1:E:24:ILE:HA	1:E:25:PRO:HD3	1.67	0.42
1:B:422:GLU:C	1:B:424:THR:H	2.28	0.42
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.77	0.42
1:C:53:LEU:HD12	1:C:53:LEU:HA	1.80	0.42
1:C:216:VAL:HG21	1:C:314:ILE:CD1	2.48	0.42
1:D:92:ALA:C	1:D:377:ASN:HD22	2.26	0.42
1:D:155:GLN:NE2	1:D:416:ARG:HB3	2.34	0.42
1:D:260:LEU:HB3	1:D:274:VAL:HG12	2.01	0.42
1:E:247:ALA:HB2	1:E:323:VAL:HG23	2.02	0.42
1:E:267:ASN:O	1:E:269:VAL:N	2.53	0.42
1:A:25:PRO:HB3	1:A:392:ASP:HB3	2.02	0.42
1:C:68:TYR:CZ	1:C:265:LEU:HD12	2.55	0.42
1:D:391:TYR:CE1	1:D:393:PRO:HG3	2.52	0.42
1:E:314:ILE:HB	1:E:315:ASN:H	1.63	0.42
1:A:68:TYR:CZ	1:A:265:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ALA:C	1:A:377:ASN:HD22	2.27	0.42
1:A:147:ASN:HA	1:A:148:PRO:HD2	1.96	0.42
1:A:376:PRO:HG3	1:A:384:MET:HE3	2.01	0.42
1:C:422:GLU:C	1:C:424:THR:H	2.28	0.42
1:A:295:SER:O	1:A:297:PRO:HD3	2.20	0.41
1:B:292:MET:HG3	1:B:334:VAL:HG22	2.02	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.83	0.41
1:B:410:ASP:HB3	1:B:423:ARG:CZ	2.47	0.41
1:A:284:ASN:OD1	1:A:284:ASN:C	2.63	0.41
1:B:267:ASN:O	1:B:269:VAL:N	2.54	0.41
1:A:422:GLU:C	1:A:424:THR:H	2.29	0.41
1:D:53:LEU:HD12	1:D:53:LEU:HA	1.80	0.41
1:D:292:MET:HG3	1:D:334:VAL:HG22	2.02	0.41
1:D:298:THR:C	1:D:300:ASN:N	2.78	0.41
1:E:168:THR:O	1:E:168:THR:OG1	2.33	0.41
1:E:298:THR:C	1:E:300:ASN:N	2.77	0.41
1:B:376:PRO:HB2	1:B:381:LEU:HD23	2.03	0.41
1:E:15:MET:C	1:E:17:PRO:HD3	2.46	0.41
1:E:292:MET:HG3	1:E:334:VAL:HG22	2.01	0.41
1:A:380:LEU:HB3	1:A:384:MET:HE2	2.02	0.41
1:C:267:ASN:O	1:C:269:VAL:N	2.53	0.41
1:C:298:THR:C	1:C:300:ASN:N	2.77	0.41
1:E:276:SER:HB2	1:E:292:MET:HE3	2.03	0.41
1:E:329:MET:HE3	1:E:329:MET:HB3	1.99	0.41
1:A:298:THR:C	1:A:300:ASN:N	2.79	0.41
1:B:185:LEU:C	1:B:187:SER:H	2.29	0.41
1:A:255:LYS:HE2	1:A:257:ASP:OD1	2.21	0.41
1:B:24:ILE:HA	1:B:25:PRO:HD3	1.67	0.41
1:C:15:MET:C	1:C:17:PRO:HD3	2.46	0.41
1:C:92:ALA:C	1:C:377:ASN:HD22	2.28	0.41
1:C:376:PRO:HG3	1:C:384:MET:HE3	2.03	0.41
1:D:147:ASN:HA	1:D:148:PRO:HD2	1.96	0.41
1:D:185:LEU:C	1:D:187:SER:H	2.29	0.41
1:D:188:MET:HB3	1:D:188:MET:HE2	1.69	0.41
1:D:214:PRO:HA	1:D:215:PRO:HD3	1.83	0.41
1:D:255:LYS:HE2	1:D:257:ASP:OD1	2.21	0.41
1:D:267:ASN:O	1:D:269:VAL:N	2.53	0.41
1:D:295:SER:O	1:D:297:PRO:HD3	2.21	0.41
1:D:412:ARG:HB2	1:D:415:TRP:CE2	2.56	0.41
1:B:168:THR:O	1:B:168:THR:OG1	2.33	0.41
1:B:214:PRO:HA	1:B:215:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ALA:HB2	1:C:323:VAL:HG23	2.02	0.41
1:E:175:VAL:HG13	1:E:340:ASN:OD1	2.21	0.41
1:E:376:PRO:HG3	1:E:384:MET:HE3	2.02	0.41
1:D:121:LEU:CD2	1:D:355:TYR:HB3	2.51	0.40
1:E:188:MET:HB3	1:E:188:MET:HE2	1.69	0.40
1:A:267:ASN:O	1:A:269:VAL:N	2.53	0.40
1:D:381:LEU:HA	1:D:381:LEU:HD23	1.85	0.40
1:E:257:ASP:OD1	1:E:277:SER:HB3	2.21	0.40
1:A:185:LEU:C	1:A:187:SER:H	2.29	0.40
1:A:292:MET:HG3	1:A:334:VAL:HG22	2.02	0.40
1:B:155:GLN:NE2	1:B:416:ARG:HB3	2.36	0.40
1:C:208:LEU:HA	1:C:209:PRO:HD3	1.83	0.40
1:D:423:ARG:HE	1:D:423:ARG:HB3	1.57	0.40
1:E:422:GLU:C	1:E:424:THR:H	2.28	0.40
1:A:24:ILE:HA	1:A:25:PRO:HD3	1.66	0.40
1:B:121:LEU:CD2	1:B:355:TYR:HB3	2.52	0.40
1:B:314:ILE:HB	1:B:315:ASN:H	1.64	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	411/442 (93%)	373 (91%)	37 (9%)	1 (0%)	43 70
1	B	412/442 (93%)	374 (91%)	37 (9%)	1 (0%)	43 70
1	C	411/442 (93%)	371 (90%)	39 (10%)	1 (0%)	43 70
1	D	412/442 (93%)	374 (91%)	37 (9%)	1 (0%)	43 70
1	E	411/442 (93%)	372 (90%)	37 (9%)	2 (0%)	24 52
All	All	2057/2210 (93%)	1864 (91%)	187 (9%)	6 (0%)	36 63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	ASP
1	C	268	ASP
1	E	268	ASP
1	B	268	ASP
1	D	268	ASP
1	E	409	LEU

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	362/385 (94%)	327 (90%)	35 (10%)	8 28
1	B	363/385 (94%)	329 (91%)	34 (9%)	8 29
1	C	362/385 (94%)	327 (90%)	35 (10%)	8 28
1	D	363/385 (94%)	330 (91%)	33 (9%)	9 30
1	E	362/385 (94%)	324 (90%)	38 (10%)	6 24
All	All	1812/1925 (94%)	1637 (90%)	175 (10%)	8 28

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	11	LEU
1	A	18	GLU
1	A	23	SER
1	A	33	ILE
1	A	34	LEU
1	A	62	SER
1	A	85	THR
1	A	125	THR
1	A	149	GLN
1	A	168	THR
1	A	175	VAL

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Mol	Chain	Res	Type
1	A	181	THR
1	A	186	GLN
1	A	194	ARG
1	A	199	ILE
1	A	212	ARG
1	A	216	VAL
1	A	219	THR
1	A	224	THR
1	A	254	THR
1	A	274	VAL
1	A	278	VAL
1	A	279	LEU
1	A	281	THR
1	A	289	SER
1	A	292	MET
1	A	294	GLN
1	A	311	SER
1	A	323	VAL
1	A	338	SER
1	A	348	ARG
1	A	370	SER
1	A	401	MET
1	A	424	THR
1	B	9	THR
1	B	11	LEU
1	B	18	GLU
1	B	23	SER
1	B	33	ILE
1	B	34	LEU
1	B	62	SER
1	B	85	THR
1	B	125	THR
1	B	149	GLN
1	B	168	THR
1	B	175	VAL
1	B	181	THR
1	B	186	GLN
1	B	194	ARG
1	B	199	ILE
1	B	212	ARG
1	B	216	VAL
1	B	219	THR

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Mol	Chain	Res	Type
1	B	224	THR
1	B	254	THR
1	B	274	VAL
1	B	278	VAL
1	B	279	LEU
1	B	281	THR
1	B	289	SER
1	B	292	MET
1	B	294	GLN
1	B	311	SER
1	B	323	VAL
1	B	338	SER
1	B	348	ARG
1	B	370	SER
1	B	424	THR
1	C	9	THR
1	C	11	LEU
1	C	18	GLU
1	C	33	ILE
1	C	34	LEU
1	C	62	SER
1	C	85	THR
1	C	125	THR
1	C	149	GLN
1	C	168	THR
1	C	175	VAL
1	C	181	THR
1	C	186	GLN
1	C	194	ARG
1	C	199	ILE
1	C	212	ARG
1	C	216	VAL
1	C	219	THR
1	C	224	THR
1	C	254	THR
1	C	263	MET
1	C	274	VAL
1	C	278	VAL
1	C	279	LEU
1	C	281	THR
1	C	289	SER
1	C	292	MET

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Mol	Chain	Res	Type
1	C	294	GLN
1	C	307	ARG
1	C	311	SER
1	C	323	VAL
1	C	338	SER
1	C	348	ARG
1	C	370	SER
1	C	424	THR
1	D	9	THR
1	D	11	LEU
1	D	18	GLU
1	D	33	ILE
1	D	34	LEU
1	D	62	SER
1	D	85	THR
1	D	125	THR
1	D	149	GLN
1	D	168	THR
1	D	175	VAL
1	D	181	THR
1	D	186	GLN
1	D	194	ARG
1	D	199	ILE
1	D	212	ARG
1	D	216	VAL
1	D	219	THR
1	D	224	THR
1	D	254	THR
1	D	274	VAL
1	D	278	VAL
1	D	279	LEU
1	D	281	THR
1	D	289	SER
1	D	292	MET
1	D	294	GLN
1	D	311	SER
1	D	323	VAL
1	D	338	SER
1	D	348	ARG
1	D	370	SER
1	D	424	THR
1	E	9	THR

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Mol	Chain	Res	Type
1	E	11	LEU
1	E	18	GLU
1	E	23	SER
1	E	33	ILE
1	E	34	LEU
1	E	62	SER
1	E	77	LEU
1	E	85	THR
1	E	125	THR
1	E	149	GLN
1	E	168	THR
1	E	175	VAL
1	E	181	THR
1	E	186	GLN
1	E	194	ARG
1	E	199	ILE
1	E	212	ARG
1	E	216	VAL
1	E	219	THR
1	E	224	THR
1	E	254	THR
1	E	263	MET
1	E	274	VAL
1	E	278	VAL
1	E	279	LEU
1	E	281	THR
1	E	289	SER
1	E	292	MET
1	E	294	GLN
1	E	307	ARG
1	E	311	SER
1	E	323	VAL
1	E	338	SER
1	E	348	ARG
1	E	370	SER
1	E	401	MET
1	E	424	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN

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Mol	Chain	Res	Type
1	A	165	ASN
1	A	183	GLN
1	A	300	ASN
1	B	74	GLN
1	B	165	ASN
1	B	183	GLN
1	B	300	ASN
1	C	74	GLN
1	C	165	ASN
1	C	183	GLN
1	D	74	GLN
1	D	165	ASN
1	E	74	GLN
1	E	165	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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	415/442 (93%)	0.27	13 (3%) 51 38	60, 104, 165, 191	0
1	B	416/442 (94%)	0.21	13 (3%) 51 38	60, 101, 164, 212	0
1	C	415/442 (93%)	0.17	11 (2%) 56 41	57, 86, 135, 177	0
1	D	416/442 (94%)	0.30	16 (3%) 44 31	56, 104, 160, 209	0
1	E	415/442 (93%)	0.04	5 (1%) 76 63	50, 78, 121, 159	0
All	All	2077/2210 (93%)	0.20	58 (2%) 55 40	50, 93, 155, 212	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	LEU	4.3
1	E	6	ALA	3.9
1	D	118	ASN	3.6
1	A	109	THR	3.5
1	C	62	SER	3.4
1	A	62	SER	3.3
1	D	207	ASP	3.3
1	C	109	THR	3.2
1	C	407	GLU	3.1
1	C	424	THR	3.1
1	D	407	GLU	3.1
1	A	426	VAL	3.0
1	C	108	SER	2.9
1	B	390	LYS	2.9
1	D	44	GLU	2.9
1	D	6	ALA	2.9
1	A	118	ASN	2.9
1	A	424	THR	2.8
1	A	407	GLU	2.8
1	D	390	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	118	ASN	2.7
1	D	408	GLU	2.7
1	D	62	SER	2.7
1	B	6	ALA	2.7
1	C	118	ASN	2.7
1	C	6	ALA	2.6
1	B	426	VAL	2.6
1	C	7	THR	2.6
1	D	127	GLU	2.5
1	A	6	ALA	2.5
1	D	146	THR	2.5
1	B	87	GLN	2.5
1	E	426	VAL	2.4
1	A	408	GLU	2.4
1	C	408	GLU	2.4
1	D	110	LEU	2.4
1	A	257	ASP	2.3
1	B	427	PHE	2.3
1	E	408	GLU	2.3
1	B	428	ASN	2.3
1	B	279	LEU	2.3
1	B	207	ASP	2.3
1	D	361	LEU	2.2
1	A	108	SER	2.2
1	E	87	GLN	2.2
1	A	61	GLY	2.2
1	C	426	VAL	2.2
1	E	407	GLU	2.2
1	D	279	LEU	2.1
1	A	87	GLN	2.1
1	D	283	ASP	2.1
1	A	427	PHE	2.1
1	D	426	VAL	2.1
1	C	106	GLN	2.0
1	B	18	GLU	2.0
1	B	295	SER	2.0
1	B	146	THR	2.0
1	D	7	THR	2.0

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

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

6.3 Carbohydrates [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(Å ²)	Q<0.9
3	CL	E	444	1/1	0.95	0.32	33,33,33,33	1
3	CL	A	444	1/1	0.96	0.08	69,69,69,69	0
2	CO	C	443	1/1	0.96	0.08	61,61,61,61	1
3	CL	C	444	1/1	0.98	0.39	34,34,34,34	1
2	CO	A	443	1/1	0.98	0.03	73,73,73,73	0
2	CO	E	443	1/1	0.99	0.07	54,54,54,54	1

6.5 Other polymers [i](#)

There are no such residues in this entry.