Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:17 PM GMT

PDB ID	:	1ERE
Title	:	HUMAN ESTROGEN RECEPTOR LIGAND-BINDING DOMAIN IN COMPLEX WITH 17BETA-ESTRADIOL
Authors	:	Brzozowski, A.M.; Pike, A.C.W.
Deposited on	:	1997-09-08
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

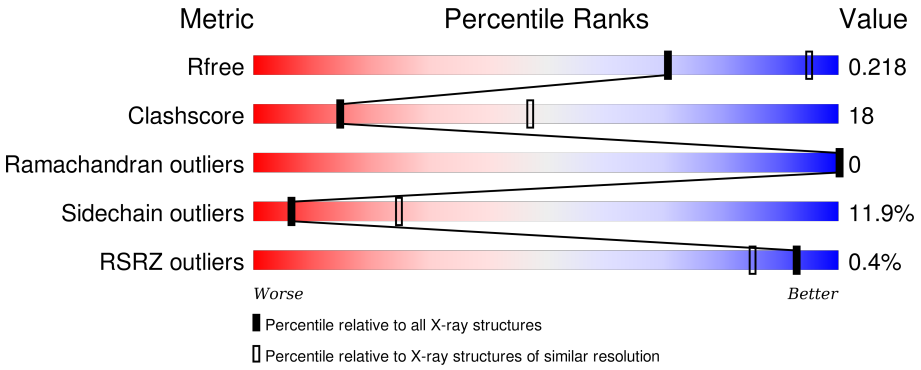
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	253	57% 29% 6% • 7%
1	B	253	% 57% 29% 6% 7%
1	C	253	56% 30% 6% • 7%
1	D	253	55% 32% 6% 7%
1	E	253	58% 28% 6% 7%

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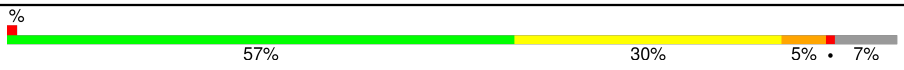
Mol	Chain	Length	Quality of chain
1	F	253	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EST	A	600	-	-	-	X
2	EST	F	600	-	-	-	X

2 Entry composition

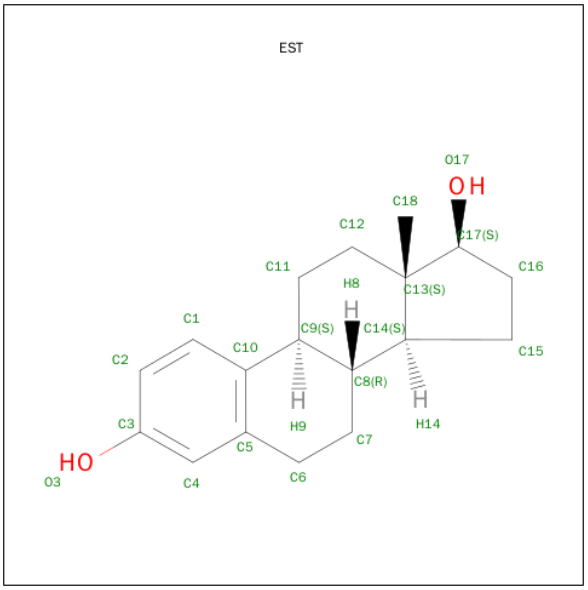
There are 3 unique types of molecules in this entry. The entry contains 11496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	B	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	C	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	D	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	E	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			
1	F	235	Total	C	N	O	S	0	5	0
			1877	1197	325	335	20			

- Molecule 2 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 20 18 2	0	0
2	B	1	Total C O 20 18 2	0	0
2	C	1	Total C O 20 18 2	0	0
2	D	1	Total C O 20 18 2	0	0
2	E	1	Total C O 20 18 2	0	0
2	F	1	Total C O 20 18 2	0	0

- Molecule 3 is water.

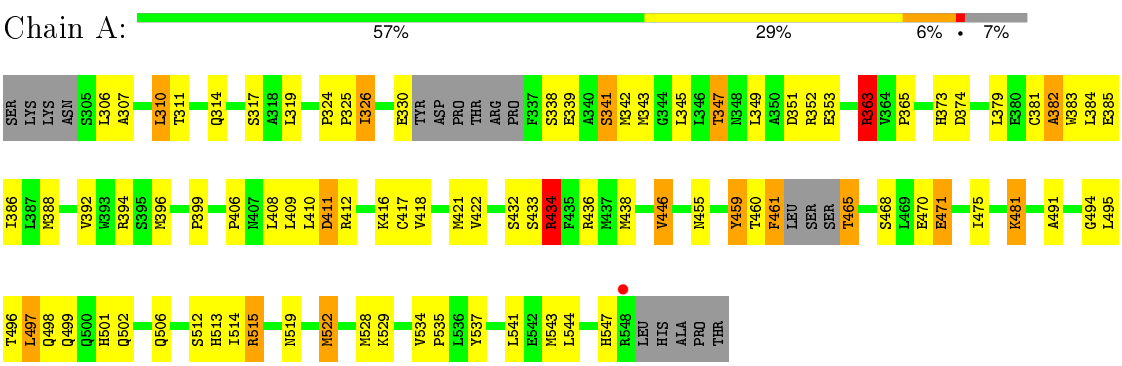
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	19	Total O 19 19	0	0
3	C	20	Total O 20 20	0	0
3	D	19	Total O 19 19	0	0
3	E	19	Total O 19 19	0	0
3	F	19	Total O 19 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

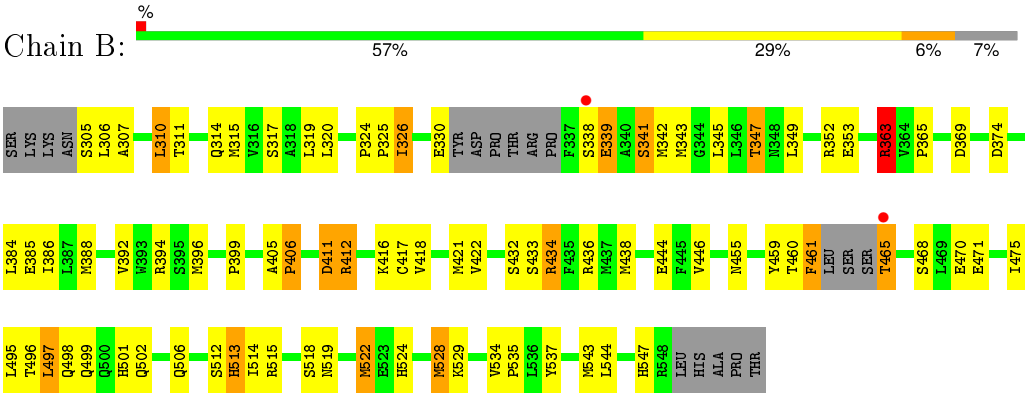
- Molecule 1: ESTROGEN RECEPTOR

Chain A:



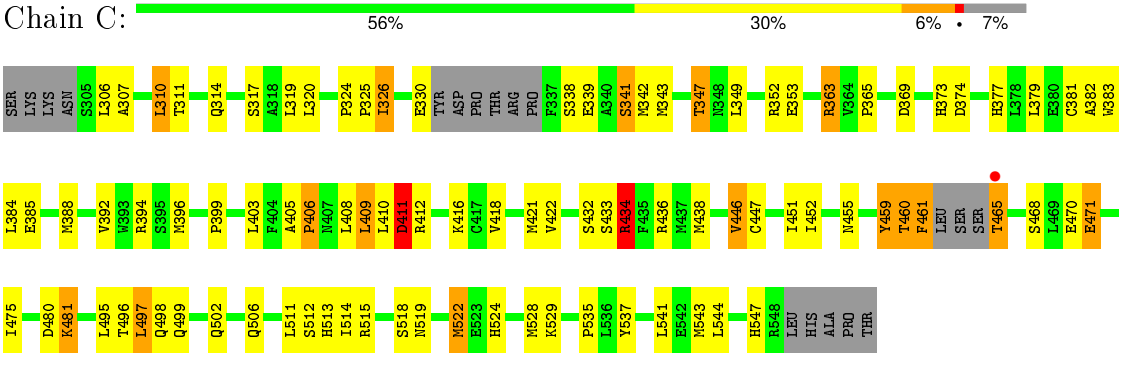
- Molecule 1: ESTROGEN RECEPTOR

Chain B:



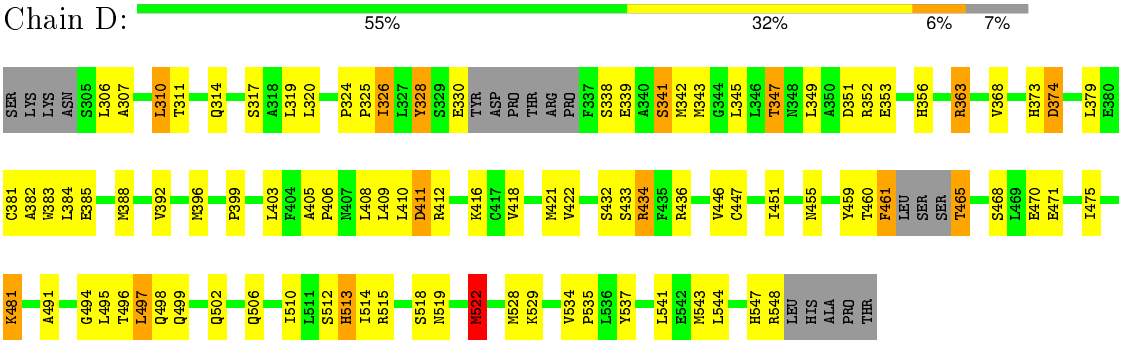
- Molecule 1: ESTROGEN RECEPTOR

Chain C:



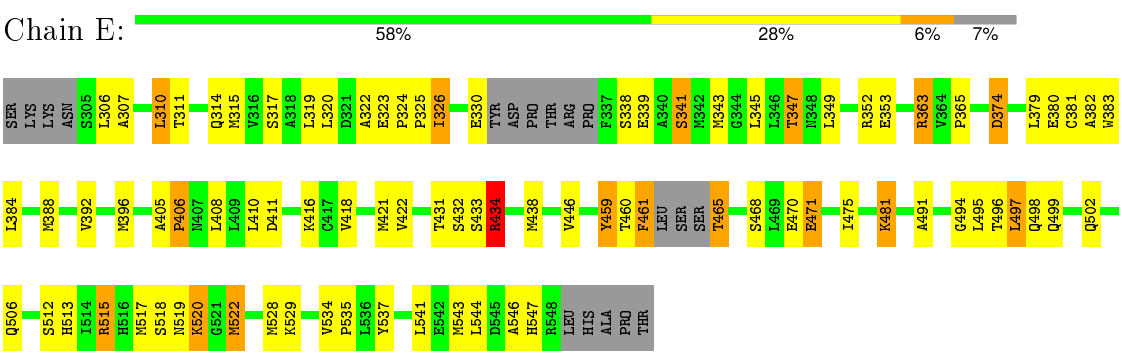
• Molecule 1: ESTROGEN RECEPTOR

Chain D:



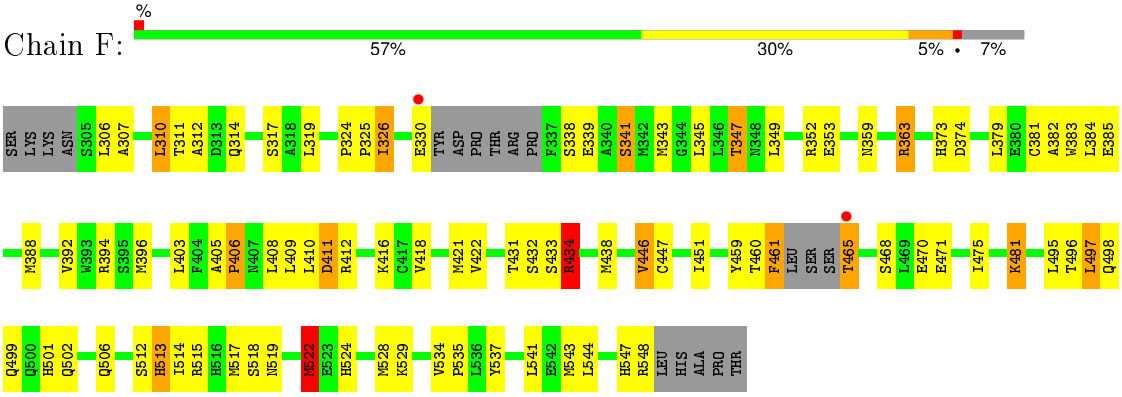
• Molecule 1: ESTROGEN RECEPTOR

Chain E:



• Molecule 1: ESTROGEN RECEPTOR

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.48Å 115.16Å 137.38Å 90.00° 98.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.10) 99.0 (19.95-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.251 0.188 , 0.218	Depositor DCC
R_{free} test set	3398 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 33981 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11496	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.57	0/1937	1.56	19/2614 (0.7%)
1	B	0.58	0/1937	1.52	16/2614 (0.6%)
1	C	0.58	0/1937	1.56	20/2614 (0.8%)
1	D	0.61	0/1937	1.55	17/2614 (0.7%)
1	E	0.58	0/1937	1.52	17/2614 (0.7%)
1	F	0.57	0/1937	1.51	18/2614 (0.7%)
All	All	0.58	0/11622	1.54	107/15684 (0.7%)

There are no bond length outliers.

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	ARG	NE-CZ-NH2	-17.34	111.63	120.30
1	B	352	ARG	NE-CZ-NH2	-16.23	112.19	120.30
1	D	352	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	C	352	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	E	352	ARG	NE-CZ-NH2	-14.05	113.28	120.30
1	F	394	ARG	NE-CZ-NH1	-12.83	113.89	120.30
1	A	394	ARG	NE-CZ-NH1	-11.88	114.36	120.30
1	A	434	ARG	NE-CZ-NH2	11.37	125.98	120.30
1	D	352	ARG	NH1-CZ-NH2	11.22	131.74	119.40
1	C	394	ARG	NE-CZ-NH1	-11.13	114.74	120.30
1	F	352	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	E	522	MET	CA-CB-CG	10.69	131.47	113.30
1	C	459	TYR	CD1-CE1-CZ	10.55	129.30	119.80
1	A	459	TYR	CD1-CE1-CZ	10.23	129.00	119.80
1	F	434	ARG	NE-CZ-NH2	10.11	125.35	120.30
1	A	522	MET	CA-CB-CG	10.09	130.45	113.30
1	E	459	TYR	CD1-CE1-CZ	9.88	128.69	119.80
1	B	434	ARG	NE-CZ-NH2	9.44	125.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	522	MET	CA-CB-CG	9.40	129.28	113.30
1	B	434	ARG	NE-CZ-NH1	-9.27	115.67	120.30
1	B	522	MET	CA-CB-CG	9.15	128.86	113.30
1	D	352	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	A	459	TYR	CB-CG-CD2	8.83	126.30	121.00
1	E	459	TYR	CB-CG-CD2	8.81	126.29	121.00
1	E	434	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	B	352	ARG	NH1-CZ-NH2	8.39	128.63	119.40
1	C	434	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	C	522	MET	CA-CB-CG	8.16	127.18	113.30
1	C	459	TYR	CB-CG-CD2	8.10	125.86	121.00
1	C	547	HIS	CA-CB-CG	-8.05	99.91	113.60
1	D	522	MET	N-CA-CB	7.88	124.78	110.60
1	D	547	HIS	CA-CB-CG	-7.80	100.34	113.60
1	E	547	HIS	CA-CB-CG	-7.76	100.41	113.60
1	C	522	MET	N-CA-CB	7.69	124.44	110.60
1	C	352	ARG	NH1-CZ-NH2	7.58	127.74	119.40
1	B	363	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	F	547	HIS	CA-CB-CG	-7.57	100.74	113.60
1	A	352	ARG	NH1-CZ-NH2	7.53	127.68	119.40
1	E	352	ARG	NH1-CZ-NH2	7.45	127.59	119.40
1	B	547	HIS	CA-CB-CG	-7.42	100.99	113.60
1	C	459	TYR	CB-CG-CD1	-7.35	116.59	121.00
1	F	522	MET	N-CA-CB	7.34	123.81	110.60
1	A	522	MET	N-CA-CB	7.19	123.54	110.60
1	F	513[A]	HIS	CA-CB-CG	-7.17	101.41	113.60
1	F	513[B]	HIS	CA-CB-CG	-7.17	101.41	113.60
1	A	459	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	D	548	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	412	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	547	HIS	CA-CB-CG	-6.97	101.74	113.60
1	E	471	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	B	522	MET	N-CA-CB	6.97	123.15	110.60
1	F	522	MET	CA-CB-CG	6.91	125.05	113.30
1	E	522	MET	N-CA-CB	6.86	122.94	110.60
1	C	480	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	406	PRO	N-CA-CB	6.81	111.47	103.30
1	A	351	ASP	CB-CG-OD1	6.80	124.42	118.30
1	E	459	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	C	394	ARG	NH1-CZ-NH2	6.77	126.85	119.40
1	B	513[A]	HIS	CA-CB-CG	-6.65	102.30	113.60
1	B	513[B]	HIS	CA-CB-CG	-6.65	102.30	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	513[A]	HIS	CA-CB-CG	-6.59	102.40	113.60
1	D	513[B]	HIS	CA-CB-CG	-6.59	102.40	113.60
1	E	382	ALA	N-CA-CB	-6.56	100.92	110.10
1	D	434	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	433	SER	N-CA-CB	-6.44	100.84	110.50
1	F	433	SER	N-CA-CB	-6.36	100.96	110.50
1	C	459	TYR	CG-CD1-CE1	-6.30	116.26	121.30
1	A	471	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	A	459	TYR	CG-CD1-CE1	-6.18	116.35	121.30
1	C	406	PRO	N-CA-CB	6.15	110.68	103.30
1	C	433	SER	N-CA-CB	-6.08	101.38	110.50
1	F	434	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	D	374	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	363	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	F	352	ARG	NH1-CZ-NH2	5.86	125.84	119.40
1	C	382	ALA	N-CA-CB	-5.81	101.97	110.10
1	F	359	ASN	CB-CG-OD1	-5.80	109.99	121.60
1	C	369	ASP	CB-CG-OD1	5.76	123.49	118.30
1	D	382	ALA	N-CA-CB	-5.64	102.21	110.10
1	B	394	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	E	406	PRO	N-CA-CB	5.61	110.04	103.30
1	E	515	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	B	369	ASP	CB-CG-OD1	5.61	123.35	118.30
1	F	394	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	D	356	HIS	CA-CB-CG	-5.57	104.14	113.60
1	E	459	TYR	CG-CD1-CE1	-5.56	116.85	121.30
1	D	328	TYR	CB-CG-CD1	-5.54	117.67	121.00
1	F	382	ALA	N-CA-CB	-5.54	102.34	110.10
1	F	406	PRO	N-CA-CB	5.41	109.79	103.30
1	C	522	MET	CB-CA-C	-5.33	99.73	110.40
1	D	433	SER	N-CA-CB	-5.33	102.51	110.50
1	A	515	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	406	PRO	N-CA-CB	5.31	109.67	103.30
1	F	522	MET	CB-CA-C	-5.29	99.81	110.40
1	C	471	GLU	OE1-CD-OE2	-5.26	116.98	123.30
1	B	433	SER	N-CA-CB	-5.21	102.69	110.50
1	A	382	ALA	N-CA-CB	-5.17	102.86	110.10
1	D	522	MET	CB-CA-C	-5.17	100.07	110.40
1	E	433	SER	N-CA-CB	-5.15	102.77	110.50
1	E	522	MET	CB-CA-C	-5.15	100.11	110.40
1	D	351	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	444	GLU	OE1-CD-OE2	5.11	129.43	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	501[A]	HIS	CA-CB-CG	5.06	122.21	113.60
1	F	501[B]	HIS	CA-CB-CG	5.06	122.21	113.60
1	A	522	MET	CB-CA-C	-5.03	100.34	110.40
1	E	374	ASP	CA-CB-CG	-5.02	102.35	113.40
1	C	411	ASP	N-CA-CB	-5.00	101.60	110.60

There are no chirality outliers.

There are no planarity outliers.

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	1877	0	1890	84	0
1	B	1877	0	1890	87	0
1	C	1877	0	1890	85	0
1	D	1877	0	1890	88	0
1	E	1877	0	1890	68	0
1	F	1877	0	1890	74	0
2	A	20	0	24	0	0
2	B	20	0	24	1	0
2	C	20	0	24	1	0
2	D	20	0	24	0	0
2	E	20	0	24	1	0
2	F	20	0	24	0	0
3	A	18	0	0	0	0
3	B	19	0	0	0	0
3	C	20	0	0	0	0
3	D	19	0	0	0	0
3	E	19	0	0	0	0
3	F	19	0	0	0	0
All	All	11496	0	11484	406	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 18.

All (406) 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:A:513[A]:HIS:CE1	1:B:459:TYR:HE1	1.13	1.65
1:E:513[A]:HIS:CE1	1:F:459:TYR:HE1	1.11	1.62
1:E:513[A]:HIS:CE1	1:F:459:TYR:CE1	1.91	1.58
1:C:513[A]:HIS:CE1	1:D:459:TYR:HE1	1.22	1.57
1:A:513[A]:HIS:CE1	1:B:459:TYR:CE1	1.96	1.52
1:C:513[A]:HIS:CE1	1:D:459:TYR:CE1	2.07	1.43
1:A:501[B]:HIS:NE2	1:B:501[B]:HIS:HE1	1.02	1.43
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:ND1	1.79	1.42
1:A:501[B]:HIS:HE1	1:B:501[B]:HIS:NE2	1.10	1.39
1:A:501[B]:HIS:ND1	1:B:501[B]:HIS:CE1	1.89	1.36
1:C:513[A]:HIS:ND1	1:D:459:TYR:CE1	1.99	1.30
1:A:513[A]:HIS:ND1	1:B:459:TYR:CE1	2.05	1.22
1:E:513[A]:HIS:ND1	1:F:459:TYR:CE1	2.03	1.22
1:A:501[B]:HIS:ND1	1:B:501[B]:HIS:ND1	1.89	1.12
1:A:497:LEU:HD11	1:B:497:LEU:HD11	1.38	1.00
1:C:519:ASN:HD22	1:D:519:ASN:HD22	1.10	0.96
1:A:373:HIS:HD2	1:C:373:HIS:HD2	0.98	0.96
1:C:513[A]:HIS:ND1	1:D:459:TYR:HE1	1.48	0.96
1:D:496:THR:HB	1:D:499:GLN:HG3	1.49	0.95
1:A:496:THR:HB	1:A:499:GLN:HG3	1.46	0.95
1:E:513[A]:HIS:HE1	1:F:459:TYR:HE1	1.08	0.94
1:D:373:HIS:HD2	1:F:373:HIS:HD2	1.09	0.93
1:E:513[A]:HIS:CE1	1:F:459:TYR:CD1	2.57	0.93
1:E:496:THR:HB	1:E:499:GLN:HG3	1.51	0.92
1:B:496:THR:HB	1:B:499:GLN:HG3	1.51	0.92
1:F:496:THR:HB	1:F:499:GLN:HG3	1.52	0.91
1:A:513[A]:HIS:HE1	1:B:459:TYR:HE1	1.18	0.90
1:C:496:THR:HB	1:C:499:GLN:HG3	1.51	0.90
1:A:373:HIS:HD2	1:C:373:HIS:CD2	1.90	0.89
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:CE1	0.88	0.88
1:A:519:ASN:HD22	1:B:519:ASN:HD22	1.22	0.87
1:C:459:TYR:HE1	1:D:513[A]:HIS:CE1	1.93	0.87
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD1	2.62	0.87
1:C:497:LEU:HD11	1:D:497:LEU:HD11	1.56	0.86
1:A:501[B]:HIS:HE1	1:B:501[B]:HIS:CE1	0.49	0.86
1:A:459:TYR:HE1	1:B:513[A]:HIS:CE1	1.95	0.85
1:D:343:MET:O	1:D:347:THR:HB	1.77	0.85
1:A:373:HIS:CD2	1:C:373:HIS:HD2	1.91	0.84
1:C:459:TYR:CE1	1:D:513[A]:HIS:CE1	2.66	0.84
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:HE1	0.53	0.83
1:E:459:TYR:HE1	1:F:513[A]:HIS:CE1	1.96	0.82
1:E:459:TYR:CE1	1:F:513[A]:HIS:CE1	2.68	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:THR:HG21	1:E:535:PRO:HD2	1.60	0.82
1:D:326:ILE:H	1:D:326:ILE:HD13	1.45	0.82
1:F:343:MET:O	1:F:347:THR:HB	1.80	0.82
1:F:347:THR:HG21	1:F:535:PRO:HD2	1.62	0.82
1:A:343:MET:O	1:A:347:THR:HB	1.81	0.81
1:A:459:TYR:CE1	1:B:513[A]:HIS:CE1	2.69	0.81
1:B:343:MET:O	1:B:347:THR:HB	1.81	0.80
1:E:497:LEU:HD11	1:F:497:LEU:HD11	1.62	0.80
1:A:347:THR:HG21	1:A:535:PRO:HD2	1.63	0.80
1:C:343:MET:O	1:C:347:THR:HB	1.82	0.79
1:E:319:LEU:HB3	1:E:446:VAL:HG13	1.64	0.79
1:A:326:ILE:H	1:A:326:ILE:HD13	1.46	0.78
1:C:347:THR:HG21	1:C:535:PRO:HD2	1.64	0.78
1:E:519:ASN:HD22	1:F:519:ASN:HD22	1.32	0.78
1:B:347:THR:HG21	1:B:535:PRO:HD2	1.65	0.76
1:D:347:THR:HG21	1:D:535:PRO:HD2	1.67	0.76
1:A:310:LEU:HB3	1:A:314:GLN:HB2	1.66	0.76
1:B:311:THR:OG1	1:B:314:GLN:HG3	1.85	0.76
1:C:513[A]:HIS:CE1	1:D:459:TYR:CD1	2.72	0.76
1:D:319:LEU:HB3	1:D:446:VAL:HG13	1.67	0.76
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.67	0.75
1:F:311:THR:OG1	1:F:314:GLN:HG3	1.87	0.75
1:A:311:THR:OG1	1:A:314:GLN:HG3	1.88	0.74
1:C:311:THR:OG1	1:C:314:GLN:HG3	1.86	0.74
1:C:326:ILE:HD13	1:C:326:ILE:H	1.52	0.73
1:C:513[A]:HIS:CD2	1:D:515:ARG:HH22	2.06	0.72
1:E:326:ILE:H	1:E:326:ILE:HD13	1.54	0.72
1:F:319:LEU:HB3	1:F:446:VAL:HG13	1.70	0.72
1:D:311:THR:OG1	1:D:314:GLN:HG3	1.90	0.72
1:B:319:LEU:HB3	1:B:446:VAL:HG13	1.71	0.71
1:E:343:MET:O	1:E:347:THR:HB	1.90	0.71
1:D:373:HIS:CD2	1:F:373:HIS:HD2	2.01	0.71
1:D:373:HIS:HD2	1:F:373:HIS:CD2	2.01	0.70
1:C:310:LEU:HB3	1:C:314:GLN:HB2	1.73	0.70
1:F:326:ILE:H	1:F:326:ILE:HD13	1.56	0.70
1:A:496:THR:CB	1:A:499:GLN:HG3	2.20	0.70
1:B:326:ILE:H	1:B:326:ILE:HD13	1.55	0.70
1:F:310:LEU:HB3	1:F:314:GLN:HB2	1.74	0.70
1:F:496:THR:CB	1:F:499:GLN:HG3	2.22	0.69
1:E:496:THR:CB	1:E:499:GLN:HG3	2.23	0.69
1:B:310:LEU:HB3	1:B:314:GLN:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:THR:CB	1:D:499:GLN:HG3	2.23	0.68
1:E:310:LEU:HB3	1:E:314:GLN:HB2	1.74	0.68
1:C:319:LEU:HB3	1:C:446:VAL:HG13	1.75	0.68
1:D:310:LEU:HB3	1:D:314:GLN:HB2	1.75	0.67
1:B:339:GLU:HA	1:B:418:VAL:HG22	1.77	0.67
1:B:496:THR:CB	1:B:499:GLN:HG3	2.23	0.66
1:A:339:GLU:HA	1:A:418:VAL:HG22	1.77	0.66
1:D:496:THR:HG22	1:D:498:GLN:H	1.60	0.65
1:E:311:THR:OG1	1:E:314:GLN:HG3	1.97	0.65
1:C:496:THR:CB	1:C:499:GLN:HG3	2.27	0.64
1:E:502:GLN:O	1:E:506[A]:GLN:HG3	1.98	0.64
1:B:418:VAL:HB	1:B:421:MET:HG3	1.80	0.64
1:F:418:VAL:HB	1:F:421:MET:HG3	1.79	0.64
1:A:459:TYR:CE1	1:B:513[A]:HIS:ND1	2.66	0.63
1:A:496:THR:HG22	1:A:498:GLN:H	1.63	0.63
1:C:513[A]:HIS:CG	1:D:459:TYR:CE1	2.86	0.63
1:F:339:GLU:HA	1:F:418:VAL:HG22	1.80	0.62
1:A:326:ILE:CD1	1:A:326:ILE:H	2.12	0.62
1:D:418:VAL:HB	1:D:421:MET:HG3	1.81	0.62
1:C:418:VAL:HB	1:C:421:MET:HG3	1.80	0.62
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:NE2	2.02	0.62
1:C:459:TYR:CE1	1:D:513[A]:HIS:ND1	2.68	0.61
1:E:496:THR:HG22	1:E:498:GLN:H	1.66	0.61
1:D:326:ILE:CD1	1:D:326:ILE:H	2.14	0.60
1:B:498:GLN:O	1:B:502:GLN:HG3	2.02	0.60
1:A:513[A]:HIS:CG	1:B:459:TYR:CE1	2.88	0.60
1:C:502:GLN:O	1:C:506[A]:GLN:HG3	2.02	0.60
1:F:522:MET:HE2	1:F:544:LEU:HD12	1.83	0.60
1:A:502:GLN:O	1:A:506[A]:GLN:HG3	2.01	0.60
1:D:495:LEU:HB3	1:D:499:GLN:HB2	1.83	0.59
1:C:326:ILE:H	1:C:326:ILE:CD1	2.15	0.59
1:E:339:GLU:HA	1:E:418:VAL:HG22	1.84	0.59
1:E:495:LEU:HB3	1:E:499:GLN:HB2	1.84	0.59
1:C:496:THR:HG22	1:C:498:GLN:H	1.67	0.59
1:E:459:TYR:CE1	1:F:513[A]:HIS:ND1	2.70	0.59
1:D:405:ALA:HB1	1:D:406:PRO:HD2	1.84	0.59
1:E:418:VAL:HB	1:E:421:MET:HG3	1.85	0.58
1:E:384:LEU:O	1:E:388:MET:HG3	2.03	0.58
1:F:502:GLN:O	1:F:506[A]:GLN:HG3	2.03	0.58
1:A:418:VAL:HB	1:A:421:MET:HG3	1.84	0.58
1:B:326:ILE:CD1	1:B:326:ILE:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HB3	1:A:499:GLN:HB2	1.86	0.57
1:C:498:GLN:O	1:C:502:GLN:HG3	2.04	0.57
1:D:502:GLN:O	1:D:506[A]:GLN:HG3	2.05	0.57
1:B:338:SER:O	1:B:339:GLU:C	2.43	0.57
1:D:339:GLU:HA	1:D:418:VAL:HG22	1.86	0.57
1:C:519:ASN:HD22	1:D:519:ASN:ND2	1.92	0.57
1:A:519:ASN:ND2	1:B:519:ASN:HD22	2.00	0.57
1:A:513[A]:HIS:NE2	1:B:459:TYR:CD1	2.73	0.57
1:B:495:LEU:HB3	1:B:499:GLN:HB2	1.87	0.57
1:C:339:GLU:HA	1:C:418:VAL:HG22	1.86	0.56
1:E:338:SER:OG	1:E:341:SER:HB3	2.06	0.56
1:E:349:LEU:O	1:E:353:GLU:HG3	2.05	0.56
1:F:374:ASP:OD2	1:F:471:GLU:OE1	2.24	0.56
1:A:338:SER:O	1:A:339:GLU:C	2.43	0.56
1:B:384:LEU:O	1:B:388:MET:HG3	2.06	0.56
1:A:501[B]:HIS:NE2	1:B:501[B]:HIS:CE1	1.95	0.55
1:E:461:PHE:HE2	1:E:475:ILE:HD12	1.72	0.55
1:F:338:SER:O	1:F:339:GLU:C	2.43	0.55
1:F:495:LEU:HB3	1:F:499:GLN:HB2	1.88	0.55
1:A:338:SER:OG	1:A:341:SER:HB3	2.07	0.55
1:A:513[A]:HIS:CD2	1:B:459:TYR:CD1	2.95	0.55
1:C:495:LEU:HB3	1:C:499:GLN:HB2	1.88	0.55
1:E:513[A]:HIS:CD2	1:F:515:ARG:HH22	2.25	0.55
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.25	0.55
1:C:522:MET:HE2	1:C:544:LEU:HD12	1.88	0.54
1:D:392:VAL:HG13	1:D:432:SER:HA	1.89	0.54
1:C:497:LEU:HD21	1:D:497:LEU:HD11	1.90	0.54
1:C:338:SER:O	1:C:339:GLU:C	2.44	0.54
1:F:384:LEU:O	1:F:388:MET:HG3	2.08	0.54
1:C:513[A]:HIS:HD2	1:D:515:ARG:HH22	1.52	0.54
1:E:513[A]:HIS:ND1	1:F:459:TYR:CD1	2.72	0.54
1:C:513[A]:HIS:HE1	1:D:455:ASN:ND2	2.06	0.54
1:F:326:ILE:H	1:F:326:ILE:CD1	2.20	0.54
1:D:328:TYR:CE1	1:D:406:PRO:HG2	2.42	0.54
1:E:383:TRP:CD1	1:E:543:MET:HB3	2.43	0.54
1:A:513[A]:HIS:CD2	1:B:515:ARG:HH22	2.24	0.53
1:F:383:TRP:CD1	1:F:543:MET:HB3	2.43	0.53
1:D:374:ASP:OD2	1:D:471:GLU:OE1	2.25	0.53
1:C:385:GLU:HG2	1:C:514:ILE:HG22	1.89	0.53
1:F:496:THR:HG22	1:F:498:GLN:H	1.73	0.53
1:F:498:GLN:O	1:F:502:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:SER:OG	1:D:341:SER:HB3	2.09	0.53
1:E:513[A]:HIS:NE2	1:F:459:TYR:CD1	2.77	0.53
1:B:392:VAL:HG13	1:B:432:SER:HA	1.91	0.53
1:A:513[A]:HIS:CG	1:B:459:TYR:CD1	2.97	0.52
1:D:311:THR:HG23	1:D:314:GLN:OE1	2.10	0.52
1:E:306:LEU:O	1:E:307:ALA:C	2.46	0.52
1:D:461:PHE:HE2	1:D:475:ILE:HD12	1.74	0.52
1:F:405:ALA:HB1	1:F:406:PRO:HD2	1.90	0.52
1:D:338:SER:O	1:D:339:GLU:C	2.45	0.52
1:D:383:TRP:HZ2	1:D:522:MET:HE1	1.75	0.52
1:A:383:TRP:HZ2	1:A:522:MET:HE1	1.74	0.52
1:C:513[A]:HIS:ND1	1:D:459:TYR:CD1	2.71	0.52
1:F:392:VAL:HG13	1:F:432:SER:HA	1.91	0.52
1:C:338:SER:OG	1:C:341:SER:HB3	2.10	0.52
1:F:349:LEU:O	1:F:353:GLU:HG3	2.10	0.52
1:B:383:TRP:CD1	1:B:543:MET:HB3	2.44	0.52
1:C:513[A]:HIS:CG	1:D:459:TYR:CD1	2.97	0.52
1:D:498:GLN:O	1:D:502:GLN:HG3	2.10	0.52
1:E:326:ILE:H	1:E:326:ILE:CD1	2.21	0.52
1:A:522:MET:HE2	1:A:544:LEU:HD12	1.92	0.52
1:B:461:PHE:HE2	1:B:475:ILE:HD12	1.75	0.51
1:A:498:GLN:O	1:A:502:GLN:HG3	2.10	0.51
1:A:311:THR:HG23	1:A:314:GLN:OE1	2.11	0.51
1:E:405:ALA:HB1	1:E:406:PRO:HD2	1.92	0.51
1:A:349:LEU:O	1:A:353:GLU:HG3	2.10	0.51
1:D:384:LEU:O	1:D:388:MET:HG3	2.10	0.51
1:E:374:ASP:OD2	1:E:471:GLU:OE1	2.29	0.51
1:B:496:THR:HG22	1:B:498:GLN:H	1.76	0.50
1:A:384:LEU:O	1:A:388:MET:HG3	2.09	0.50
1:A:496:THR:HG22	1:A:497:LEU:N	2.25	0.50
1:C:497:LEU:HD11	1:D:497:LEU:HD21	1.92	0.50
1:B:363:ARG:HG3	1:B:363:ARG:NH1	2.25	0.50
1:E:338:SER:O	1:E:339:GLU:C	2.49	0.50
1:E:522:MET:HE2	1:E:544:LEU:HD12	1.93	0.50
1:E:498:GLN:O	1:E:502:GLN:HG3	2.11	0.50
1:D:408:LEU:HD11	1:D:410:LEU:HD21	1.93	0.50
1:E:311:THR:HG23	1:E:314:GLN:OE1	2.12	0.50
1:B:306:LEU:O	1:B:307:ALA:C	2.50	0.50
1:B:405:ALA:HB1	1:B:406:PRO:HD2	1.93	0.50
1:E:497:LEU:HD21	1:F:497:LEU:HD11	1.93	0.50
1:D:306:LEU:O	1:D:307:ALA:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:TYR:O	1:C:541:LEU:HG	2.12	0.50
1:C:349:LEU:O	1:C:353:GLU:HG3	2.12	0.50
1:D:522:MET:HE2	1:D:544:LEU:HD12	1.94	0.49
1:B:496:THR:HG22	1:B:497:LEU:N	2.26	0.49
1:B:374:ASP:OD2	1:B:471:GLU:OE1	2.28	0.49
1:C:405:ALA:HB1	1:C:406:PRO:HD2	1.94	0.49
1:A:513[A]:HIS:ND1	1:B:459:TYR:CD1	2.76	0.49
1:E:513[A]:HIS:CG	1:F:459:TYR:CE1	2.95	0.49
1:C:515:ARG:HH22	1:D:513[A]:HIS:CD2	2.30	0.49
1:C:383:TRP:CD1	1:C:543:MET:HB3	2.47	0.49
1:B:522:MET:HE2	1:B:544:LEU:HD12	1.95	0.49
1:A:461:PHE:HE2	1:A:475:ILE:HD12	1.77	0.49
1:F:306:LEU:O	1:F:307:ALA:C	2.51	0.49
1:C:497:LEU:HD11	1:D:497:LEU:CD1	2.36	0.49
1:F:385:GLU:HG2	1:F:514:ILE:HG22	1.94	0.49
1:F:535:PRO:HG2	1:F:537:TYR:CE2	2.48	0.48
1:B:311:THR:HG23	1:B:314:GLN:OE1	2.13	0.48
1:A:382:ALA:O	1:A:386:ILE:HG12	2.13	0.48
1:B:502:GLN:O	1:B:506[A]:GLN:HG3	2.13	0.48
1:A:491:ALA:O	1:A:494:GLY:N	2.38	0.48
1:B:535:PRO:HG2	1:B:537:TYR:CE2	2.48	0.48
1:D:349:LEU:O	1:D:353:GLU:HG3	2.13	0.48
1:F:405:ALA:HB1	1:F:406:PRO:CD	2.44	0.48
1:F:465:THR:O	1:F:468:SER:HB2	2.14	0.48
1:C:461:PHE:HE2	1:C:475:ILE:HD12	1.78	0.48
1:E:465:THR:O	1:E:468:SER:HB2	2.14	0.48
1:A:383:TRP:CD1	1:A:543:MET:HB3	2.49	0.48
1:B:342:MET:HE2	1:B:417:CYS:HB2	1.96	0.48
1:A:399:PRO:HA	1:A:436:ARG:NH2	2.28	0.48
1:D:405:ALA:HB1	1:D:406:PRO:CD	2.43	0.48
1:B:385:GLU:HG2	1:B:514:ILE:HG22	1.96	0.48
1:F:411:ASP:O	1:F:412:ARG:C	2.52	0.48
1:A:385:GLU:HG2	1:A:514:ILE:HG22	1.96	0.48
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.32	0.47
1:C:392:VAL:HG13	1:C:432:SER:HA	1.95	0.47
1:F:496:THR:HG22	1:F:497:LEU:N	2.29	0.47
1:B:310:LEU:O	1:B:481:LYS:HE3	2.14	0.47
1:B:383:TRP:HZ2	1:B:522:MET:HE1	1.79	0.47
1:E:513[A]:HIS:CG	1:F:459:TYR:CD1	3.03	0.47
1:D:326:ILE:HD13	1:D:326:ILE:N	2.21	0.47
1:B:382:ALA:O	1:B:386:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LEU:O	1:C:388:MET:HG3	2.13	0.47
1:C:496:THR:HG22	1:C:497:LEU:N	2.30	0.47
1:E:496:THR:HG22	1:E:497:LEU:N	2.30	0.47
1:A:515:ARG:HH22	1:B:513[A]:HIS:CD2	2.32	0.47
1:A:310:LEU:O	1:A:481:LYS:HE3	2.15	0.47
1:E:491:ALA:O	1:E:494:GLY:N	2.39	0.47
1:F:338:SER:OG	1:F:341:SER:HB3	2.15	0.47
1:D:324:PRO:HB2	1:D:325:PRO:HD2	1.97	0.47
1:E:363:ARG:NH1	1:E:363:ARG:HG3	2.29	0.47
1:F:434:ARG:O	1:F:438:MET:HG3	2.14	0.47
1:A:306:LEU:O	1:A:307:ALA:C	2.53	0.46
1:D:403:LEU:CD1	1:D:409:LEU:HD22	2.45	0.46
1:E:497:LEU:HD11	1:F:497:LEU:HD21	1.97	0.46
1:E:535:PRO:HG2	1:E:537:TYR:CE2	2.50	0.46
1:F:319:LEU:CB	1:F:446:VAL:HG13	2.43	0.46
1:D:310:LEU:O	1:D:481:LYS:HE3	2.15	0.46
1:D:383:TRP:CD1	1:D:543:MET:HB3	2.50	0.46
1:C:306:LEU:O	1:C:307:ALA:C	2.53	0.46
1:C:363:ARG:O	1:C:365:PRO:HD3	2.16	0.46
1:C:519:ASN:ND2	1:D:519:ASN:HD22	1.93	0.46
1:A:465:THR:O	1:A:468:SER:HB2	2.15	0.46
1:E:380:GLU:HB3	1:E:546:ALA:CB	2.45	0.46
1:A:459:TYR:CD1	1:A:459:TYR:N	2.84	0.46
1:B:315:MET:HE3	1:B:365:PRO:HG2	1.97	0.46
1:C:513[A]:HIS:CE1	1:D:455:ASN:O	2.69	0.46
1:C:497:LEU:CD1	1:D:497:LEU:HD11	2.36	0.46
1:F:311:THR:HG23	1:F:314:GLN:OE1	2.15	0.46
1:C:405:ALA:HB1	1:C:406:PRO:CD	2.46	0.46
1:D:379:LEU:HA	1:D:379:LEU:HD23	1.85	0.46
1:F:408:LEU:HD11	1:F:410:LEU:HD21	1.97	0.46
1:C:408:LEU:HD11	1:C:410:LEU:HD21	1.98	0.46
1:C:434:ARG:O	1:C:438:MET:HG3	2.16	0.46
1:B:528:MET:HB3	1:B:534:VAL:HG23	1.98	0.45
1:B:349:LEU:O	1:B:353:GLU:HG3	2.16	0.45
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.88	0.45
1:A:324:PRO:CB	1:A:325:PRO:HD2	2.47	0.45
1:E:392:VAL:HG13	1:E:432:SER:HA	1.98	0.45
1:C:513[A]:HIS:NE2	1:D:455:ASN:O	2.48	0.45
1:D:535:PRO:HG2	1:D:537:TYR:CE2	2.51	0.45
1:B:465:THR:O	1:B:468:SER:HB2	2.17	0.45
1:B:411:ASP:O	1:B:412:ARG:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:TYR:CD1	1:C:459:TYR:N	2.85	0.45
1:A:363:ARG:HG3	1:A:363:ARG:NH1	2.30	0.45
1:D:363:ARG:NH1	1:D:363:ARG:HG3	2.32	0.45
1:A:408:LEU:HD11	1:A:410:LEU:HD21	1.97	0.45
1:C:465:THR:O	1:C:468:SER:HB2	2.16	0.45
1:F:383:TRP:HZ2	1:F:522:MET:HE1	1.80	0.45
1:E:315:MET:HE1	1:E:365:PRO:HB2	1.98	0.45
1:C:455:ASN:ND2	1:D:513[A]:HIS:HE1	2.13	0.45
1:A:342:MET:HE2	1:A:417:CYS:HB2	1.99	0.45
1:A:537:TYR:O	1:A:541:LEU:HG	2.17	0.45
1:A:319:LEU:CB	1:A:446:VAL:HG13	2.44	0.45
1:F:363:ARG:HG3	1:F:363:ARG:NH1	2.31	0.45
1:B:324:PRO:HB2	1:B:325:PRO:HD2	1.98	0.45
1:D:342:MET:HE2	1:D:418:VAL:HG23	1.99	0.45
1:B:324:PRO:CB	1:B:325:PRO:HD2	2.47	0.45
1:C:447:CYS:O	1:C:451:ILE:HG13	2.17	0.45
1:E:513[A]:HIS:CD2	1:F:459:TYR:CD1	3.05	0.44
1:F:324:PRO:CB	1:F:325:PRO:HD2	2.47	0.44
1:A:324:PRO:HB2	1:A:325:PRO:HD2	1.98	0.44
1:C:320:LEU:HD23	1:C:320:LEU:HA	1.79	0.44
1:F:431:THR:OG1	1:F:517:MET:HE1	2.17	0.44
1:F:537:TYR:O	1:F:541:LEU:HG	2.16	0.44
1:C:535:PRO:HG2	1:C:537:TYR:CE2	2.53	0.44
1:E:461:PHE:CE2	1:E:475:ILE:HD12	2.51	0.44
1:E:408:LEU:HD11	1:E:410:LEU:HD21	1.99	0.44
1:B:338:SER:OG	1:B:341:SER:HB3	2.17	0.44
1:F:403:LEU:HD12	1:F:409:LEU:HD22	1.99	0.44
1:D:399:PRO:HA	1:D:436:ARG:NH2	2.33	0.44
1:F:461:PHE:HE2	1:F:475:ILE:HD12	1.82	0.44
1:C:363:ARG:NH1	1:C:363:ARG:HG3	2.33	0.44
1:F:528:MET:HB3	1:F:534:VAL:HG23	1.98	0.44
1:A:535:PRO:HG2	1:A:537:TYR:CE2	2.52	0.44
1:F:403:LEU:CD1	1:F:409:LEU:HD22	2.48	0.44
1:E:459:TYR:N	1:E:459:TYR:CD1	2.85	0.44
1:E:537:TYR:O	1:E:541:LEU:HG	2.17	0.44
1:B:347:THR:CG2	1:B:537:TYR:HE2	2.31	0.44
1:D:461:PHE:HA	1:D:461:PHE:HD1	1.61	0.44
1:B:461:PHE:CE2	1:B:475:ILE:HD12	2.53	0.44
1:E:434:ARG:O	1:E:438:MET:HG3	2.18	0.44
1:D:324:PRO:CB	1:D:325:PRO:HD2	2.47	0.43
1:E:528:MET:HB3	1:E:534:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:THR:O	1:D:468:SER:HB2	2.18	0.43
1:C:403:LEU:HD12	1:C:409:LEU:HD22	2.00	0.43
1:E:405:ALA:HB1	1:E:406:PRO:CD	2.48	0.43
1:D:411:ASP:O	1:D:412:ARG:C	2.56	0.43
1:D:528:MET:HB3	1:D:534:VAL:HG23	2.01	0.43
1:A:411:ASP:O	1:A:412:ARG:C	2.56	0.43
1:A:392:VAL:HG13	1:A:432:SER:HA	2.00	0.43
1:D:392:VAL:HG13	1:D:432:SER:CA	2.47	0.43
1:E:320:LEU:HA	1:E:320:LEU:HD23	1.71	0.43
1:E:310:LEU:O	1:E:481:LYS:HE3	2.18	0.43
1:A:461:PHE:CE2	1:A:475:ILE:HD12	2.53	0.43
1:B:524:HIS:CE1	1:B:528:MET:HG2	2.53	0.43
1:C:379:LEU:HA	1:C:379:LEU:HD23	1.84	0.43
1:D:447:CYS:O	1:D:451:ILE:HG13	2.19	0.43
1:C:411:ASP:O	1:C:412:ARG:C	2.55	0.43
1:E:520:LYS:H	1:E:520:LYS:HG2	1.61	0.43
1:A:434:ARG:O	1:A:438:MET:HG3	2.18	0.43
1:B:434:ARG:O	1:B:438:MET:HG3	2.19	0.43
1:B:305:SER:O	1:B:306:LEU:C	2.57	0.42
1:A:455:ASN:ND2	1:B:513[A]:HIS:HE1	2.16	0.42
1:D:491:ALA:O	1:D:494:GLY:N	2.43	0.42
1:C:497:LEU:HD21	1:D:497:LEU:CD1	2.49	0.42
1:D:461:PHE:CE2	1:D:475:ILE:HD12	2.53	0.42
1:E:431:THR:OG1	1:E:517:MET:HE1	2.19	0.42
1:A:528:MET:HB3	1:A:534:VAL:HG23	2.01	0.42
1:C:452:ILE:HD11	1:C:511:LEU:HD22	2.01	0.42
1:F:379:LEU:HA	1:F:379:LEU:HD23	1.84	0.42
1:F:324:PRO:HB2	1:F:325:PRO:HD2	2.00	0.42
1:F:311:THR:O	1:F:312:ALA:C	2.58	0.42
1:E:383:TRP:HZ2	1:E:522:MET:HE1	1.85	0.42
1:D:385:GLU:HG2	1:D:514:ILE:HG22	2.02	0.42
1:D:320:LEU:HA	1:D:320:LEU:HD23	1.76	0.42
1:D:537:TYR:O	1:D:541:LEU:HG	2.20	0.41
1:B:405:ALA:HB1	1:B:406:PRO:CD	2.49	0.41
1:C:399:PRO:HA	1:C:436:ARG:NH2	2.35	0.41
1:B:399:PRO:HA	1:B:436:ARG:NH2	2.34	0.41
2:E:600:EST:H181	2:E:600:EST:H152	1.85	0.41
1:C:497:LEU:CD1	1:D:497:LEU:HD21	2.51	0.41
1:C:324:PRO:CB	1:C:325:PRO:HD2	2.50	0.41
1:F:310:LEU:O	1:F:481:LYS:HE3	2.21	0.41
1:B:461:PHE:HD1	1:B:461:PHE:HA	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ARG:H	1:C:363:ARG:HG2	1.46	0.41
1:A:363:ARG:O	1:A:365:PRO:HD3	2.20	0.41
1:E:515:ARG:HH22	1:F:513[A]:HIS:CD2	2.37	0.41
2:C:600:EST:H181	2:C:600:EST:H152	1.75	0.41
1:F:522:MET:HB3	1:F:522:MET:HE2	1.96	0.41
1:B:363:ARG:H	1:B:363:ARG:HG2	1.55	0.41
1:A:347:THR:CG2	1:A:537:TYR:HE2	2.34	0.41
1:C:347:THR:CG2	1:C:537:TYR:HE2	2.33	0.41
1:C:310:LEU:O	1:C:481:LYS:HE3	2.20	0.41
1:D:342:MET:CE	1:D:418:VAL:HG23	2.50	0.41
1:C:524:HIS:CE1	1:C:528:MET:HG2	2.56	0.41
1:B:347:THR:HG22	1:B:537:TYR:HE2	1.84	0.41
1:B:522:MET:HB3	1:B:522:MET:HE2	1.99	0.41
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.74	0.41
1:B:379:LEU:HA	1:B:379:LEU:HD23	1.96	0.41
1:D:328:TYR:HE1	1:D:406:PRO:HB2	1.86	0.41
1:A:513[A]:HIS:HE1	1:B:455:ASN:ND2	2.19	0.41
1:D:496:THR:HG22	1:D:497:LEU:N	2.36	0.41
1:F:347:THR:HG21	1:F:535:PRO:CD	2.44	0.41
1:B:486:LEU:HA	1:B:486:LEU:HD23	1.93	0.41
1:E:322:ALA:O	1:E:323:GLU:C	2.59	0.41
1:D:434:ARG:HG2	1:D:510:ILE:HD11	2.03	0.40
1:E:379:LEU:HA	1:E:379:LEU:HD23	1.87	0.40
1:C:461:PHE:CE2	1:C:475:ILE:HD12	2.56	0.40
1:C:403:LEU:CD1	1:C:409:LEU:HD22	2.51	0.40
1:E:324:PRO:HB2	1:E:325:PRO:HD2	2.02	0.40
1:C:342:MET:CE	1:C:418:VAL:HG23	2.51	0.40
1:C:377[A]:HIS:NE2	1:C:460:THR:O	2.54	0.40
1:D:534:VAL:HA	1:D:535:PRO:HD3	1.96	0.40
1:C:342:MET:HE2	1:C:418:VAL:HG23	2.04	0.40
1:F:524:HIS:CE1	1:F:528:MET:HG2	2.55	0.40
2:B:600:EST:H182	2:B:600:EST:H111	1.91	0.40
1:F:447:CYS:O	1:F:451:ILE:HG13	2.21	0.40
1:B:347:THR:HG23	1:B:537:TYR:CD2	2.56	0.40
1:A:436:ARG:HH11	1:A:436:ARG:HD2	1.75	0.40
1:B:436:ARG:HH11	1:B:436:ARG:HD2	1.75	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	234/253 (92%)	223 (95%)	11 (5%)	0	100	100
1	B	234/253 (92%)	225 (96%)	9 (4%)	0	100	100
1	C	234/253 (92%)	226 (97%)	8 (3%)	0	100	100
1	D	234/253 (92%)	227 (97%)	7 (3%)	0	100	100
1	E	234/253 (92%)	225 (96%)	9 (4%)	0	100	100
1	F	234/253 (92%)	224 (96%)	10 (4%)	0	100	100
All	All	1404/1518 (92%)	1350 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	210/228 (92%)	186 (89%)	24 (11%)	7	28
1	B	210/228 (92%)	186 (89%)	24 (11%)	7	28
1	C	210/228 (92%)	186 (89%)	24 (11%)	7	28
1	D	210/228 (92%)	186 (89%)	24 (11%)	7	28
1	E	210/228 (92%)	186 (89%)	24 (11%)	7	28
1	F	210/228 (92%)	184 (88%)	26 (12%)	6	23
All	All	1260/1368 (92%)	1114 (88%)	146 (12%)	6	27

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	317	SER
1	A	326	ILE
1	A	330	GLU
1	A	341	SER
1	A	345	LEU
1	A	347	THR
1	A	363	ARG
1	A	381	CYS
1	A	396	MET
1	A	409	LEU
1	A	411	ASP
1	A	416	LYS
1	A	422	VAL
1	A	434	ARG
1	A	446	VAL
1	A	460	THR
1	A	461	PHE
1	A	465	THR
1	A	470	GLU
1	A	481	LYS
1	A	497	LEU
1	A	512	SER
1	A	529	LYS
1	B	310	LEU
1	B	317	SER
1	B	326	ILE
1	B	330	GLU
1	B	339	GLU
1	B	341	SER
1	B	345	LEU
1	B	347	THR
1	B	363	ARG
1	B	381	CYS
1	B	396	MET
1	B	411	ASP
1	B	416	LYS
1	B	422	VAL
1	B	460	THR
1	B	461	PHE
1	B	465	THR
1	B	470	GLU

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Mol	Chain	Res	Type
1	B	481	LYS
1	B	497	LEU
1	B	512	SER
1	B	518	SER
1	B	528	MET
1	B	529	LYS
1	C	310	LEU
1	C	317	SER
1	C	326	ILE
1	C	330	GLU
1	C	341	SER
1	C	347	THR
1	C	363	ARG
1	C	381	CYS
1	C	396	MET
1	C	409	LEU
1	C	411	ASP
1	C	416	LYS
1	C	422	VAL
1	C	434	ARG
1	C	446	VAL
1	C	460	THR
1	C	461	PHE
1	C	465	THR
1	C	470	GLU
1	C	481	LYS
1	C	497	LEU
1	C	512	SER
1	C	518	SER
1	C	529	LYS
1	D	310	LEU
1	D	317	SER
1	D	326	ILE
1	D	330	GLU
1	D	341	SER
1	D	345	LEU
1	D	347	THR
1	D	363	ARG
1	D	368	VAL
1	D	381	CYS
1	D	396	MET
1	D	411	ASP

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Mol	Chain	Res	Type
1	D	416	LYS
1	D	422	VAL
1	D	460	THR
1	D	461	PHE
1	D	465	THR
1	D	470	GLU
1	D	481	LYS
1	D	497	LEU
1	D	512	SER
1	D	518	SER
1	D	522	MET
1	D	529	LYS
1	E	310	LEU
1	E	317	SER
1	E	326	ILE
1	E	330	GLU
1	E	341	SER
1	E	345	LEU
1	E	347	THR
1	E	363	ARG
1	E	381	CYS
1	E	396	MET
1	E	411	ASP
1	E	416	LYS
1	E	422	VAL
1	E	434	ARG
1	E	460	THR
1	E	461	PHE
1	E	465	THR
1	E	470	GLU
1	E	481	LYS
1	E	497	LEU
1	E	512	SER
1	E	518	SER
1	E	520	LYS
1	E	529	LYS
1	F	310	LEU
1	F	317	SER
1	F	326	ILE
1	F	330	GLU
1	F	341	SER
1	F	345	LEU

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Mol	Chain	Res	Type
1	F	347	THR
1	F	363	ARG
1	F	381	CYS
1	F	396	MET
1	F	411	ASP
1	F	416	LYS
1	F	422	VAL
1	F	434	ARG
1	F	446	VAL
1	F	460	THR
1	F	461	PHE
1	F	465	THR
1	F	470	GLU
1	F	481	LYS
1	F	497	LEU
1	F	512	SER
1	F	518	SER
1	F	522	MET
1	F	529	LYS
1	F	548	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	A	439	ASN
1	A	455	ASN
1	A	519	ASN
1	B	439	ASN
1	B	455	ASN
1	C	373	HIS
1	C	439	ASN
1	C	455	ASN
1	D	373	HIS
1	D	439	ASN
1	D	455	ASN
1	D	519	ASN
1	E	439	ASN
1	E	455	ASN
1	F	373	HIS
1	F	439	ASN
1	F	455	ASN

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Mol	Chain	Res	Type
1	F	519	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EST	A	600	-	23,23,23	0.81	0	36,36,36	1.97	12 (33%)
2	EST	B	600	-	23,23,23	1.02	1 (4%)	36,36,36	1.85	10 (27%)
2	EST	C	600	-	23,23,23	0.92	0	36,36,36	1.66	7 (19%)
2	EST	D	600	-	23,23,23	1.10	2 (8%)	36,36,36	2.03	10 (27%)
2	EST	E	600	-	23,23,23	1.01	2 (8%)	36,36,36	1.85	9 (25%)
2	EST	F	600	-	23,23,23	1.05	2 (8%)	36,36,36	1.99	9 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EST	A	600	-	-	0/0/40/40	0/4/4/4
2	EST	B	600	-	-	0/0/40/40	0/4/4/4
2	EST	C	600	-	-	0/0/40/40	0/4/4/4
2	EST	D	600	-	-	0/0/40/40	0/4/4/4
2	EST	E	600	-	-	0/0/40/40	0/4/4/4
2	EST	F	600	-	-	0/0/40/40	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	EST	C10-C9	-2.30	1.48	1.52
2	D	600	EST	C8-C14	-2.27	1.49	1.53
2	B	600	EST	C8-C14	-2.17	1.49	1.53
2	E	600	EST	C10-C9	-2.14	1.49	1.52
2	E	600	EST	C8-C14	-2.07	1.49	1.53
2	F	600	EST	C8-C14	-2.05	1.49	1.53
2	F	600	EST	C10-C9	-2.05	1.49	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	EST	C15-C16-C17	-4.51	101.30	105.75
2	F	600	EST	C3-C4-C5	-4.44	116.16	120.75
2	D	600	EST	C3-C4-C5	-4.41	116.18	120.75
2	C	600	EST	C15-C14-C13	-4.41	98.08	103.82
2	E	600	EST	C3-C4-C5	-4.28	116.32	120.75
2	E	600	EST	C15-C14-C13	-4.14	98.44	103.82
2	A	600	EST	C15-C14-C13	-4.12	98.46	103.82
2	B	600	EST	C3-C4-C5	-3.88	116.74	120.75
2	F	600	EST	C11-C12-C13	-3.84	105.98	112.84
2	A	600	EST	C15-C16-C17	-3.82	101.98	105.75
2	E	600	EST	C16-C15-C14	-3.71	97.65	105.12
2	B	600	EST	C11-C12-C13	-3.69	106.25	112.84
2	A	600	EST	C3-C4-C5	-3.59	117.04	120.75
2	F	600	EST	C15-C16-C17	-3.57	102.22	105.75
2	A	600	EST	C11-C12-C13	-3.54	106.52	112.84
2	E	600	EST	C11-C12-C13	-3.52	106.56	112.84
2	C	600	EST	C11-C12-C13	-3.50	106.58	112.84
2	F	600	EST	C16-C15-C14	-3.42	98.25	105.12
2	B	600	EST	C15-C16-C17	-3.32	102.47	105.75
2	F	600	EST	C15-C14-C13	-3.30	99.53	103.82
2	C	600	EST	C12-C11-C9	-3.19	108.47	112.20
2	D	600	EST	C15-C14-C13	-3.09	99.81	103.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	EST	C11-C12-C13	-2.88	107.69	112.84
2	E	600	EST	C15-C16-C17	-2.79	102.99	105.75
2	B	600	EST	C15-C14-C13	-2.79	100.19	103.82
2	C	600	EST	C15-C16-C17	-2.70	103.09	105.75
2	A	600	EST	C16-C15-C14	-2.59	99.91	105.12
2	A	600	EST	C12-C11-C9	-2.53	109.25	112.20
2	C	600	EST	C3-C4-C5	-2.47	118.20	120.75
2	B	600	EST	C12-C11-C9	-2.44	109.36	112.20
2	E	600	EST	C12-C11-C9	-2.43	109.36	112.20
2	A	600	EST	C1-C2-C3	-2.42	117.07	119.87
2	D	600	EST	C16-C15-C14	-2.41	100.27	105.12
2	C	600	EST	C16-C15-C14	-2.37	100.35	105.12
2	D	600	EST	C6-C5-C4	-2.32	115.25	119.84
2	A	600	EST	C13-C14-C8	-2.21	110.92	114.37
2	E	600	EST	C6-C5-C4	-2.14	115.61	119.84
2	D	600	EST	C12-C11-C9	-2.04	109.82	112.20
2	F	600	EST	C6-C5-C4	-2.04	115.81	119.84
2	A	600	EST	C9-C8-C14	-2.03	105.81	108.88
2	B	600	EST	C6-C5-C4	-2.02	115.85	119.84
2	B	600	EST	C16-C15-C14	-2.00	101.09	105.12
2	C	600	EST	C12-C13-C14	2.13	110.78	107.31
2	D	600	EST	O17-C17-C13	2.23	119.39	114.78
2	A	600	EST	C12-C13-C14	2.30	111.05	107.31
2	E	600	EST	C2-C3-C4	2.55	123.12	120.19
2	E	600	EST	C16-C17-C13	2.71	106.68	104.58
2	F	600	EST	C12-C13-C14	2.77	111.80	107.31
2	B	600	EST	C2-C3-C4	2.85	123.46	120.19
2	B	600	EST	O17-C17-C13	3.02	121.01	114.78
2	D	600	EST	C2-C3-C4	3.46	124.16	120.19
2	F	600	EST	C2-C3-C4	3.60	124.33	120.19
2	A	600	EST	C2-C3-C4	3.81	124.57	120.19
2	A	600	EST	C16-C17-C13	3.93	107.63	104.58
2	F	600	EST	C16-C17-C13	4.05	107.73	104.58
2	B	600	EST	C16-C17-C13	4.32	107.94	104.58
2	D	600	EST	C16-C17-C13	6.31	109.48	104.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	EST	1	0
2	C	600	EST	1	0
2	E	600	EST	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	235/253 (92%)	-0.49	1 (0%)	93	85	36, 55, 88, 128	0
1	B	235/253 (92%)	-0.45	2 (0%)	85	72	37, 55, 88, 128	0
1	C	235/253 (92%)	-0.48	1 (0%)	93	85	35, 55, 88, 128	0
1	D	235/253 (92%)	-0.47	0	100	100	34, 54, 87, 128	0
1	E	235/253 (92%)	-0.51	0	100	100	35, 54, 87, 128	0
1	F	235/253 (92%)	-0.48	2 (0%)	85	72	36, 55, 87, 128	0
All	All	1410/1518 (92%)	-0.48	6 (0%)	93	85	34, 55, 88, 128	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	THR	3.4
1	B	338	SER	3.4
1	C	465	THR	3.1
1	F	465	THR	2.7
1	A	548	ARG	2.3
1	F	330	GLU	2.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	EST	A	600	20/20	0.98	0.28	3.12	34,35,38,40	0
2	EST	F	600	20/20	0.97	0.24	2.78	33,35,38,40	0
2	EST	D	600	20/20	0.97	0.24	1.48	32,34,38,39	0
2	EST	C	600	20/20	0.97	0.20	1.18	35,35,38,38	0
2	EST	B	600	20/20	0.97	0.18	0.96	33,35,39,40	0
2	EST	E	600	20/20	0.97	0.19	0.49	33,34,38,40	0

6.5 Other polymers (i)

There are no such residues in this entry.