



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:38 AM GMT

PDB ID : 3FF6
Title : Human ACC2 CT domain with CP-640186
Authors : Williams, S.P.; Madauss, K.P.; Burkhart, W.A.
Deposited on : 2008-12-02
Resolution : 3.19 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

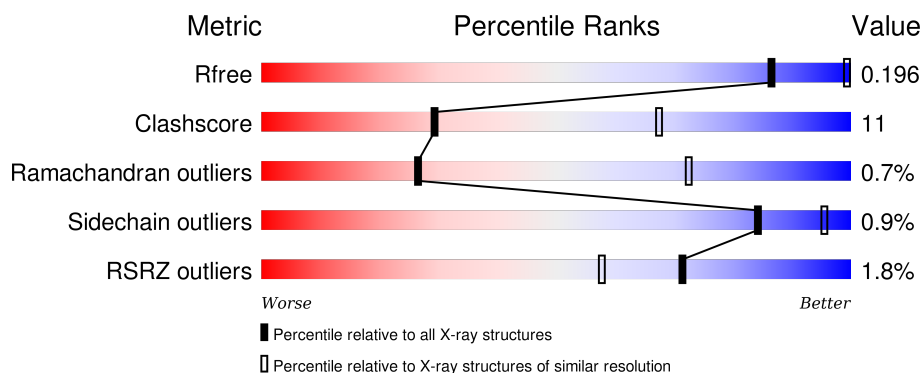
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. 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	760	<div> <div>2%</div> <div>78% 20% ..</div> </div>
1	B	760	<div> <div>%</div> <div>75% 23% .</div> </div>
1	C	760	<div> <div>3%</div> <div>77% 20% ..</div> </div>
1	D	760	<div> <div>%</div> <div>74% 22% ..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22989 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.

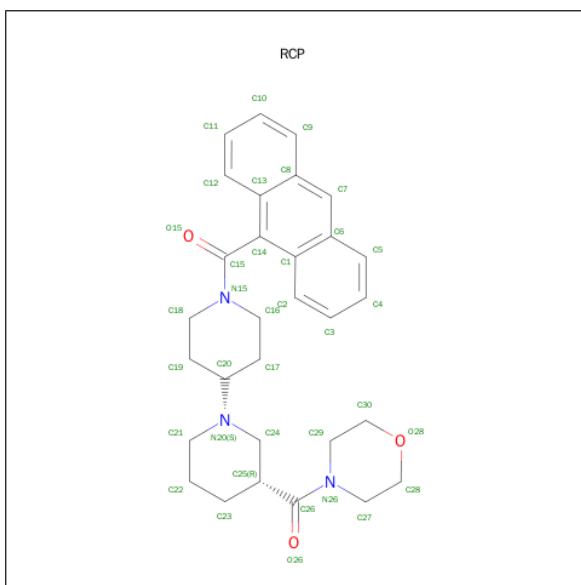
- Molecule 1 is a protein called Acetyl-CoA carboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			5656	3628	961	1044	23			
1	B	748	Total	C	N	O	S	0	0	0
			5754	3684	988	1058	24			
1	C	742	Total	C	N	O	S	0	0	0
			5706	3650	980	1052	24			
1	D	733	Total	C	N	O	S	0	0	0
			5641	3615	965	1037	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1692	GLY	-	EXPRESSION TAG	UNP O00763
A	2451	GLU	-	EXPRESSION TAG	UNP O00763
B	1692	GLY	-	EXPRESSION TAG	UNP O00763
B	2451	GLU	-	EXPRESSION TAG	UNP O00763
C	1692	GLY	-	EXPRESSION TAG	UNP O00763
C	2451	GLU	-	EXPRESSION TAG	UNP O00763
D	1692	GLY	-	EXPRESSION TAG	UNP O00763
D	2451	GLU	-	EXPRESSION TAG	UNP O00763

- Molecule 2 is (3R)-1'-(9-ANTHRYLCARBONYL)-3-(MORPHOLIN-4-YLCARBONYL)-1, 4'-BIPIPERIDINE (three-letter code: RCP) (formula: C₃₀H₃₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	30	3	3		
2	B	1	Total	C	N	O	0	0
			36	30	3	3		
2	C	1	Total	C	N	O	0	0
			36	30	3	3		
2	D	1	Total	C	N	O	0	0
			36	30	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	28	Total	O	0	0
			28	28		
3	C	16	Total	O	0	0
			16	16		
3	D	21	Total	O	0	0
			21	21		

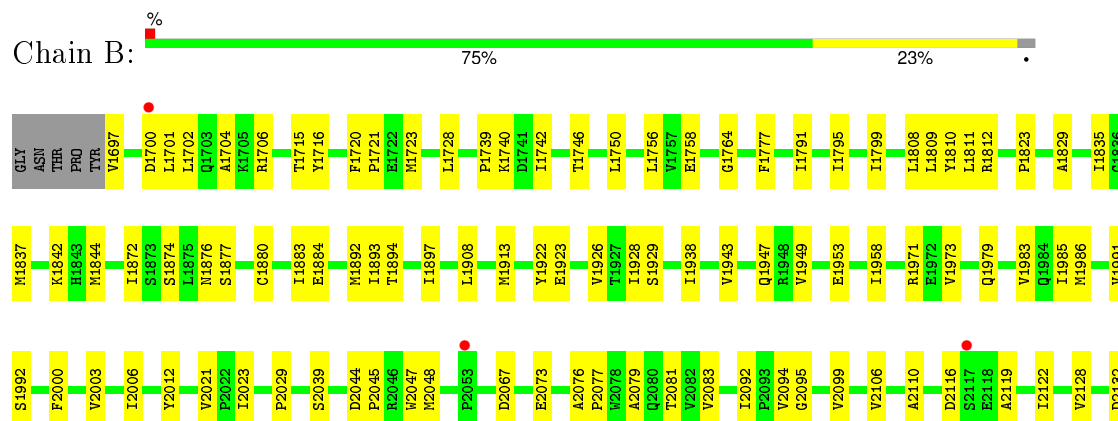
3 Residue-property plots

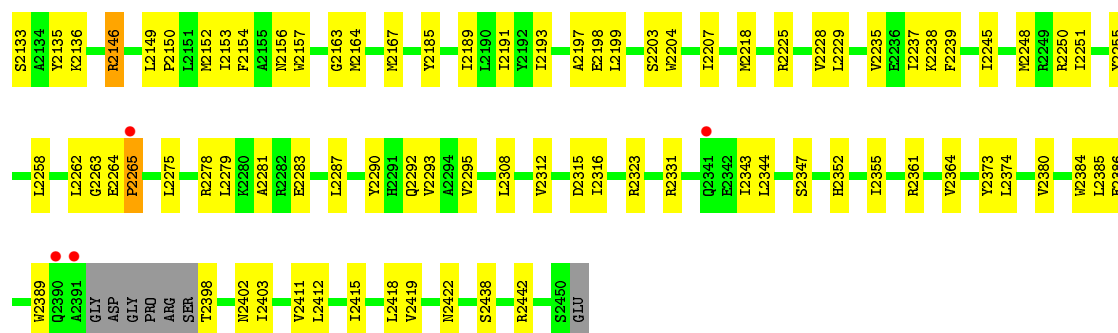
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Acetyl-CoA carboxylase 2

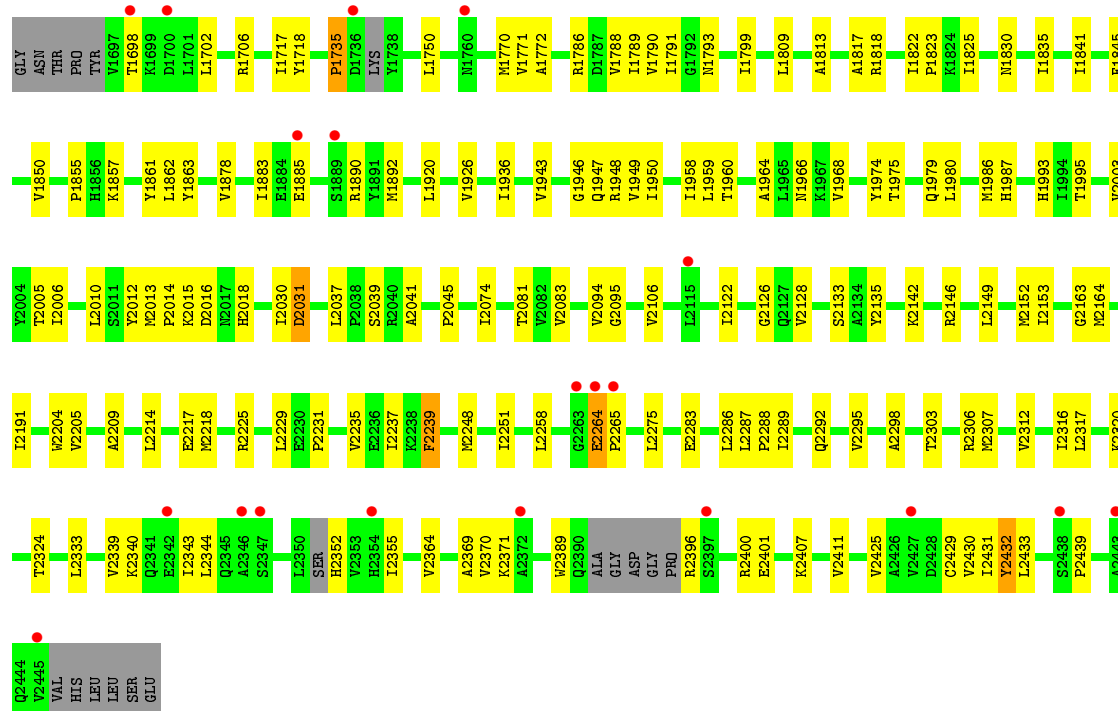
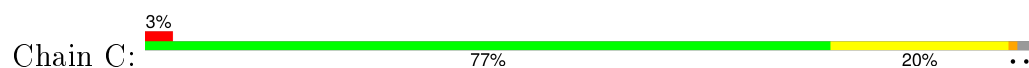


• Molecule 1: Acetyl-CoA carboxylase 2

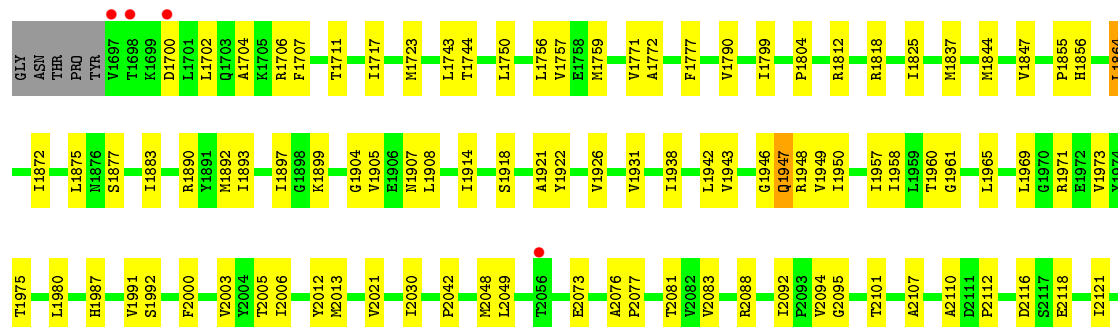




• Molecule 1: Acetyl-CoA carboxylase 2



• Molecule 1: Acetyl-CoA carboxylase 2



H2388	L2286	V2128
H2389	L2287	W2129
Q2390	L2288	S2133
A2391	L2289	R2146
GLY	H2291	L2149
ASP	Q2292	P2150
GLY	L2293	L2151
L2396	A2294	W2152
S2397	V2295	L2153
K2407	T2303	F2154
V2411	R2306	A2155
R2416	V2312	F2160
V2419	L2317	G2163
W2422	T2324	W2167
L2433	R2331	L2182
SER	R2332	L2189
GLN	L2333	L2190
HIS	I2334	L2191
ILE	Q2341	V2192
SER	E2342	L2193
PRO	Q2345	E2198
ALA	A2346	L2199
GLU	S2347	R2200
ARG	G2348	W2204
ALA	L2350	L2207
GLN	E2349	L2217
VAL	L2351	M2218
VAL	H2352	Y2219
HIS	L2353	S2224
LEU	R2354	V2228
SER	L2355	V2235
LEU	Q2356	F2236
SER	S2357	L2237
GLU	W2362	R2238
	T2366	F2239
	V2373	D2252
	L2374	L2262
	W2375	D2271
	N2378	L2275
	V2381	L2278
	V2382	
	Q2383	
	W2384	
	L2385	
	E2386	
	Q2387	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.55Å 168.84Å 293.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.19 20.00 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-3.19) 94.5 (20.00-3.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.197 , 0.251 0.205 , 0.196	Depositor DCC
R_{free} test set	4652 reflections (7.79%)	DCC
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 64397 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22989	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: RCP

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	0.41	1/5788 (0.0%)	0.54	1/7896 (0.0%)
1	B	0.39	0/5890	0.55	0/8012
1	C	0.38	0/5839	0.54	2/7949 (0.0%)
1	D	0.39	0/5775	0.53	0/7865
All	All	0.39	1/23292 (0.0%)	0.54	3/31722 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2438	SER	CB-OG	9.19	1.54	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1735	PRO	N-CA-CB	6.16	110.69	103.30
1	A	1695	PRO	N-CA-CB	5.34	109.70	103.30
1	C	2031	ASP	CB-CG-OD2	5.24	123.01	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5656	0	5369	141	0
1	B	5754	0	5528	146	0
1	C	5706	0	5470	138	0
1	D	5641	0	5414	145	0
2	A	36	0	35	3	0
2	B	36	0	35	2	0
2	C	36	0	35	1	0
2	D	36	0	35	1	0
3	A	23	0	0	0	0
3	B	28	0	0	0	0
3	C	16	0	0	0	0
3	D	21	0	0	1	0
All	All	22989	0	21921	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 11.

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:D:2030:ILE:O	1:D:2324:THR:HG22	1.43	1.18
1:B:1723:MET:CE	1:B:2000:PHE:HA	1.89	1.02
1:A:2343:ILE:HG22	1:A:2403:ILE:HG21	1.38	1.02
1:A:1723:MET:CE	1:A:2000:PHE:HA	1.94	0.97
1:A:2191:ILE:HD13	1:A:2207:ILE:HG22	1.48	0.96
1:D:1723:MET:HE3	1:D:2000:PHE:HA	1.47	0.94
1:D:1883:ILE:HD12	1:D:1892:MET:HE3	1.48	0.94
1:A:2343:ILE:CG2	1:A:2403:ILE:HG21	1.97	0.93
1:B:1883:ILE:HD12	1:B:1892:MET:HE3	1.46	0.93
1:A:1723:MET:HE3	1:A:2000:PHE:HA	1.51	0.92
1:C:2030:ILE:O	1:C:2324:THR:HG22	1.70	0.91
1:B:2308:LEU:HD12	1:B:2316:ILE:HG23	1.52	0.90
1:C:2010:LEU:HD23	1:C:2013:MET:CE	2.01	0.90
1:C:2344:LEU:HD23	1:C:2355:ILE:HG23	1.54	0.89
1:A:1791:ILE:CD1	1:A:1813:ALA:HB1	2.03	0.89
1:C:2344:LEU:CD2	1:C:2355:ILE:HG23	2.02	0.89
1:A:1791:ILE:HD11	1:A:1813:ALA:HB1	1.53	0.89
1:C:2214:LEU:HD21	1:C:2352:HIS:NE2	1.87	0.88
1:C:1841:ILE:HD12	1:C:1878:VAL:HG21	1.54	0.88
1:A:2164:MET:HE3	1:B:1979:GLN:O	1.74	0.87
1:C:2153:ILE:HD12	1:C:2191:ILE:CD1	2.04	0.87
1:C:1772:ALA:HB1	1:C:1791:ILE:HG22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2153:ILE:HD12	1:C:2191:ILE:HD13	1.59	0.84
1:A:2191:ILE:HD13	1:A:2207:ILE:CG2	2.08	0.84
1:C:1835:ILE:HG22	1:D:2228:VAL:HG11	1.61	0.83
1:A:2343:ILE:HG21	1:A:2403:ILE:HD13	1.59	0.82
1:A:2030:ILE:O	1:A:2324:THR:HG22	1.79	0.81
1:D:1883:ILE:HD12	1:D:1892:MET:CE	2.09	0.81
1:C:2010:LEU:HD23	1:C:2013:MET:HE3	1.59	0.81
1:A:2344:LEU:HD23	1:A:2355:ILE:HG23	1.63	0.80
1:A:2164:MET:HE3	1:B:1985:ILE:HD11	1.62	0.80
1:B:1701:LEU:HD21	1:B:1764:GLY:HA3	1.62	0.80
1:D:2081:THR:HG21	1:D:2128:VAL:O	1.80	0.80
1:B:2081:THR:HG21	1:B:2128:VAL:O	1.82	0.79
1:A:1835:ILE:HG22	1:B:2228:VAL:HG11	1.65	0.79
1:A:2343:ILE:CG2	1:A:2403:ILE:HD13	2.13	0.78
1:C:2094:VAL:HG21	1:C:2152:MET:HG3	1.64	0.78
1:C:1772:ALA:CB	1:C:1791:ILE:HG22	2.15	0.77
1:C:1788:VAL:HG21	1:C:1825:ILE:HD13	1.66	0.77
1:D:2351:SER:CB	1:D:2354:HIS:HB2	2.16	0.76
1:C:2214:LEU:HD21	1:C:2352:HIS:CE1	2.21	0.75
1:B:2067:ASP:OD1	1:B:2323:ARG:NH2	2.19	0.75
1:C:2010:LEU:HA	1:C:2013:MET:HE2	1.70	0.74
1:C:2214:LEU:HD21	1:C:2352:HIS:HE2	1.51	0.74
1:B:2263:GLY:C	1:B:2265:PRO:HD3	2.08	0.74
1:A:2081:THR:HG21	1:A:2128:VAL:O	1.87	0.73
1:B:2153:ILE:HD12	1:B:2191:ILE:CD1	2.18	0.73
1:C:1791:ILE:HG21	1:C:1813:ALA:HB1	1.71	0.73
1:C:2258:LEU:HD22	1:C:2275:LEU:HD22	1.70	0.73
1:C:2163:GLY:HA2	1:D:1980:LEU:HD22	1.70	0.73
1:C:2312:VAL:HG21	1:D:1905:VAL:HG12	1.69	0.73
1:D:1926:VAL:HG21	1:D:2013:MET:HE2	1.72	0.72
1:D:1723:MET:CE	1:D:2000:PHE:HA	2.20	0.72
1:C:1862:LEU:HD21	1:D:2293:VAL:HG23	1.72	0.72
1:D:1931:VAL:HG21	1:D:1957:ILE:HD11	1.70	0.72
1:B:1723:MET:HE3	1:B:2000:PHE:HA	1.70	0.72
1:C:1788:VAL:CG2	1:C:1825:ILE:HD13	2.20	0.71
1:C:1789:ILE:HD12	1:C:1817:ALA:HB2	1.72	0.71
1:A:2029:PRO:O	1:A:2323:ARG:NH1	2.23	0.71
1:B:2283:GLU:O	1:B:2287:LEU:HD13	1.88	0.71
1:A:2343:ILE:HG22	1:A:2403:ILE:CG2	2.19	0.71
1:A:1723:MET:HE3	1:A:2000:PHE:CA	2.21	0.71
1:A:2010:LEU:HA	1:A:2013:MET:HE2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1926:VAL:CG2	1:D:2013:MET:HE2	2.20	0.70
1:A:2422:ASN:ND2	1:B:2411:VAL:HG21	2.06	0.70
1:A:2164:MET:CE	1:B:1985:ILE:HD11	2.22	0.70
1:B:2229:LEU:HD11	1:B:2237:ILE:HD12	1.73	0.69
1:C:2081:THR:HG21	1:C:2128:VAL:O	1.91	0.69
1:B:2248:MET:HE1	1:B:2283:GLU:HB2	1.74	0.69
1:D:2362:TRP:O	1:D:2366:THR:HG23	1.93	0.68
1:B:2116:ASP:OD2	1:C:2041:ALA:HB2	1.93	0.68
1:D:2110:ALA:HB2	1:D:2118:GLU:HA	1.75	0.68
1:A:2335:LEU:HB3	1:A:2385:LEU:HD13	1.75	0.68
1:A:1702:LEU:HD21	1:A:1706:ARG:NH2	2.09	0.67
1:B:1723:MET:HE3	1:B:2000:PHE:CA	2.23	0.67
1:B:1823:PRO:HB3	1:B:1926:VAL:HG13	1.77	0.67
1:A:1883:ILE:CD1	1:A:1892:MET:HE3	2.25	0.67
1:C:1966:ASN:HD21	1:C:1974:TYR:H	1.41	0.67
1:D:2235:VAL:HG13	1:D:2239:PHE:HB3	1.76	0.66
1:A:1880:CYS:HB3	1:A:1893:ILE:HA	1.77	0.66
1:D:1949:VAL:HG11	1:D:1991:VAL:O	1.94	0.66
1:A:2289:ILE:HD12	1:D:1975:THR:HG21	1.77	0.66
1:B:2106:VAL:HG13	1:B:2122:ILE:HB	1.78	0.66
1:A:2080:GLN:HB2	1:A:2104:VAL:HG11	1.77	0.66
1:A:2010:LEU:HD23	1:A:2013:MET:HE3	1.77	0.66
1:D:2218:MET:HE3	1:D:2312:VAL:O	1.96	0.66
1:A:1926:VAL:HG11	1:A:2013:MET:HE1	1.77	0.65
1:B:2153:ILE:HD12	1:B:2191:ILE:HD12	1.78	0.65
1:B:1791:ILE:HD11	1:B:1810:TYR:HA	1.78	0.65
1:A:2344:LEU:CD2	1:A:2355:ILE:HG23	2.26	0.65
1:B:2094:VAL:HG21	1:B:2152:MET:HG3	1.78	0.65
1:C:2344:LEU:HD21	1:C:2355:ILE:HG23	1.79	0.65
1:C:2106:VAL:HG13	1:C:2122:ILE:HB	1.78	0.64
1:A:1791:ILE:HD12	1:A:1813:ALA:CB	2.27	0.64
1:A:2010:LEU:HD23	1:A:2013:MET:CE	2.28	0.64
1:B:1883:ILE:HD12	1:B:1892:MET:CE	2.26	0.64
1:C:1835:ILE:HD11	1:D:2237:ILE:HG21	1.80	0.63
1:C:1980:LEU:HD22	1:D:2163:GLY:HA2	1.80	0.63
1:B:2203:SER:O	1:B:2207:ILE:HG22	1.98	0.63
1:D:1949:VAL:CG1	1:D:1991:VAL:O	2.47	0.62
1:C:2396:ARG:HA	1:C:2400:ARG:CB	2.29	0.62
1:C:1790:VAL:HG22	1:C:1825:ILE:HB	1.80	0.62
1:A:1791:ILE:CD1	1:A:1813:ALA:CB	2.76	0.62
1:B:2343:ILE:HG22	1:B:2403:ILE:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1841:ILE:HD12	1:C:1878:VAL:CG2	2.26	0.62
1:A:1723:MET:HE1	1:A:2000:PHE:HA	1.82	0.61
1:C:2433:LEU:HD22	1:D:2419:VAL:HG21	1.81	0.61
1:A:2099:VAL:HG22	1:A:2157:TRP:CE2	2.36	0.61
1:B:2331:ARG:NH2	1:B:2386:GLU:OE2	2.34	0.61
1:C:2081:THR:HB	1:C:2133:SER:OG	2.00	0.61
1:A:1883:ILE:HD12	1:A:1892:MET:HE3	1.81	0.61
1:D:1914:ILE:HD12	1:D:1942:LEU:HD11	1.83	0.61
1:A:1926:VAL:HG11	1:A:2013:MET:CE	2.31	0.61
1:C:2003:VAL:HA	1:C:2006:ILE:HD12	1.82	0.61
1:A:1845:PHE:O	1:B:2250:ARG:NH2	2.33	0.61
1:D:2388:HIS:O	1:D:2397:SER:HA	2.00	0.60
1:B:1953:GLU:HA	1:B:1983:VAL:HG21	1.82	0.60
1:C:1926:VAL:HG21	1:C:2013:MET:CE	2.31	0.60
1:D:2153:ILE:HD12	1:D:2191:ILE:CD1	2.31	0.60
1:C:2225:ARG:HH12	1:C:2303:THR:HG22	1.67	0.60
1:A:1985:ILE:HD11	1:B:2164:MET:HG3	1.83	0.60
1:A:2419:VAL:HG13	1:A:2426:ALA:HB2	1.83	0.60
1:B:1876:ASN:O	1:B:1876:ASN:CG	2.39	0.60
1:C:2225:ARG:NH1	1:C:2303:THR:HG22	2.16	0.60
1:B:1728:LEU:HD11	1:B:1777:PHE:CB	2.31	0.60
1:D:2081:THR:HB	1:D:2133:SER:OG	2.02	0.60
1:B:1723:MET:CE	1:B:2000:PHE:CA	2.72	0.60
1:A:1979:GLN:O	1:B:2164:MET:HE3	2.02	0.59
1:D:2182:LEU:HD22	1:D:2189:ILE:HD13	1.85	0.59
1:A:2411:VAL:HG13	1:B:2418:LEU:HD13	1.83	0.59
1:C:2343:ILE:HD13	1:C:2389:TRP:CE2	2.38	0.59
1:B:2290:TYR:O	1:B:2293:VAL:HG12	2.02	0.59
1:C:2286:LEU:HD21	1:D:1855:PRO:HG2	1.84	0.59
1:B:1949:VAL:HG13	1:B:1992:SER:HA	1.84	0.59
1:B:2343:ILE:HG22	1:B:2403:ILE:CD1	2.32	0.59
1:B:1811:LEU:HD22	1:B:1913:MET:SD	2.43	0.59
1:D:2378:ASN:O	1:D:2382:VAL:HG23	2.02	0.59
1:C:1789:ILE:HG13	1:C:1822:ILE:HD11	1.84	0.59
1:A:1779:THR:HG23	1:A:1782:TYR:H	1.68	0.59
1:B:2081:THR:HB	1:B:2133:SER:OG	2.02	0.58
1:A:1850:VAL:HG12	1:A:1858:GLY:O	2.03	0.58
1:C:1786:ARG:HB2	1:C:2015:LYS:HG3	1.85	0.58
1:C:2433:LEU:CD2	1:D:2419:VAL:HG21	2.34	0.58
1:D:2073:GLU:OE2	1:D:2083:VAL:HG13	2.03	0.58
1:C:2235:VAL:HG13	1:C:2239:PHE:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2041:ALA:HB2	1:D:2116:ASP:OD2	2.03	0.58
1:A:1717:ILE:HG12	1:A:1771:VAL:HG22	1.86	0.58
1:D:2048:MET:HE3	1:D:2049:LEU:HD12	1.85	0.57
1:A:1958:ILE:HA	1:B:2167:MET:HE2	1.85	0.57
1:C:1791:ILE:HG21	1:C:1813:ALA:CB	2.34	0.57
1:C:2343:ILE:HD13	1:C:2389:TRP:CZ2	2.39	0.57
1:C:1950:ILE:HD13	1:C:2005:THR:HB	1.85	0.57
1:A:1953:GLU:HA	1:A:1983:VAL:HG21	1.87	0.57
1:A:1841:ILE:HD13	1:A:1844:MET:SD	2.44	0.57
1:C:1698:THR:HA	1:C:1702:LEU:HB3	1.87	0.56
1:A:2388:HIS:CB	1:A:2399:ILE:CG2	2.84	0.56
1:B:1728:LEU:HD11	1:B:1777:PHE:HB2	1.87	0.56
1:C:1946:GLY:O	1:C:1948:ARG:N	2.37	0.56
1:A:2344:LEU:HD23	1:A:2355:ILE:CG2	2.36	0.56
1:B:2116:ASP:CG	1:C:2041:ALA:HB2	2.25	0.56
1:A:2204:TRP:CB	1:B:1908:LEU:HD13	2.36	0.56
1:C:2235:VAL:HG21	1:C:2295:VAL:HG12	1.86	0.55
1:D:2355:ILE:HG22	1:D:2356:GLN:N	2.21	0.55
1:C:1855:PRO:HB2	1:D:2289:ILE:HD11	1.88	0.55
1:A:2081:THR:CG2	1:A:2128:VAL:O	2.54	0.55
1:B:2343:ILE:CG2	1:B:2403:ILE:HD12	2.37	0.55
1:A:2422:ASN:HD22	1:B:2411:VAL:HG21	1.70	0.55
1:A:2387:GLN:HE21	1:A:2398:THR:HG21	1.72	0.55
1:C:1835:ILE:CG2	1:D:2228:VAL:HG11	2.36	0.54
1:C:1986:MET:HE1	1:D:2167:MET:CE	2.37	0.54
1:D:2303:THR:HG23	1:D:2306:ARG:H	1.71	0.54
1:C:2340:LYS:HG3	1:C:2355:ILE:HG22	1.90	0.54
1:C:2106:VAL:CG1	1:C:2122:ILE:HB	2.37	0.54
1:D:1750:LEU:HD23	1:D:1756:LEU:HD23	1.89	0.54
1:D:2107:ALA:HA	1:D:2121:ILE:HG22	1.90	0.54
1:A:1947:GLN:O	1:A:1949:VAL:HG23	2.08	0.54
1:B:2343:ILE:HG21	1:B:2403:ILE:HD12	1.89	0.54
1:A:2204:TRP:HB3	1:B:1908:LEU:HD13	1.90	0.54
1:B:1723:MET:HE3	1:B:2000:PHE:N	2.23	0.54
1:D:2218:MET:CE	1:D:2312:VAL:O	2.56	0.53
1:B:2343:ILE:HG13	1:B:2389:TRP:CZ2	2.43	0.53
1:A:2415:ILE:HG23	1:B:2415:ILE:HD12	1.91	0.53
1:C:2411:VAL:HG21	1:D:2422:ASN:ND2	2.23	0.53
1:A:1818:ARG:HD3	1:A:1921:ALA:HA	1.89	0.53
1:A:1846:HIS:HA	1:B:2251:ILE:HD11	1.89	0.53
1:C:1883:ILE:HG21	1:C:1892:MET:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2364:VAL:HG13	1:C:2369:ALA:HA	1.89	0.53
1:B:1823:PRO:CB	1:B:1926:VAL:HG13	2.39	0.53
1:B:1715:THR:HG22	1:B:1716:TYR:O	2.08	0.53
1:A:2418:LEU:O	1:A:2422:ASN:N	2.37	0.53
1:B:1697:VAL:O	1:B:1701:LEU:N	2.42	0.53
1:C:2312:VAL:HG21	1:D:1905:VAL:CG1	2.36	0.53
1:C:2204:TRP:HB3	1:D:1908:LEU:HD13	1.91	0.53
1:C:1823:PRO:HB3	1:C:1926:VAL:HG13	1.91	0.52
1:A:2278:ARG:O	1:A:2281:ALA:HB3	2.09	0.52
1:B:1880:CYS:HB3	1:B:1893:ILE:HA	1.90	0.52
1:A:1960:THR:HG21	2:B:2:RCP:H171	1.90	0.52
1:D:2353:VAL:HG23	1:D:2354:HIS:CD2	2.44	0.52
1:A:2415:ILE:HG12	1:B:2415:ILE:HD13	1.91	0.52
1:C:2030:ILE:C	1:C:2030:ILE:HD12	2.30	0.52
1:B:1884:GLU:OE1	1:B:1884:GLU:N	2.42	0.52
1:A:2081:THR:HB	1:A:2133:SER:OG	2.09	0.52
1:A:1883:ILE:HD13	1:A:1892:MET:HE3	1.91	0.52
1:B:1746:THR:HG21	1:B:1758:GLU:OE1	2.10	0.52
1:C:1770:MET:HG2	1:C:1793:ASN:HA	1.92	0.52
1:D:1973:VAL:HG12	1:D:2112:PRO:HB2	1.92	0.52
1:C:2407:LYS:O	1:C:2411:VAL:HG23	2.10	0.52
1:A:1793:ASN:HD22	1:A:1829:ALA:H	1.57	0.52
1:D:1723:MET:HE3	1:D:2000:PHE:CA	2.29	0.51
1:B:2229:LEU:CD1	1:B:2237:ILE:HD12	2.39	0.51
1:B:2343:ILE:HG13	1:B:2389:TRP:HZ2	1.74	0.51
1:B:2079:ALA:HB2	1:B:2132:ASP:HB2	1.92	0.51
1:B:1723:MET:HE1	1:B:2000:PHE:HA	1.86	0.51
1:B:1971:ARG:NH1	1:B:1973:VAL:HG22	2.26	0.51
1:D:2347:SER:HB2	1:D:2407:LYS:HA	1.91	0.51
1:D:2353:VAL:O	1:D:2357:SER:CB	2.59	0.51
1:D:1947:GLN:O	1:D:1949:VAL:HG12	2.10	0.51
1:D:2262:LEU:CD1	1:D:2279:LEU:HD22	2.40	0.51
1:B:1723:MET:HE2	1:B:2000:PHE:HA	1.88	0.51
1:B:2248:MET:HE1	1:B:2283:GLU:CB	2.39	0.51
1:D:2110:ALA:CB	1:D:2118:GLU:HA	2.41	0.51
1:A:2232:GLU:HG2	2:A:1:RCP:C4	2.41	0.51
1:A:2194:PRO:HD2	1:A:2197:ALA:CB	2.41	0.51
1:A:1791:ILE:HD12	1:A:1813:ALA:HB1	1.81	0.51
1:C:2264:GLU:CB	1:C:2265:PRO:CD	2.88	0.51
1:A:2012:TYR:OH	1:A:2070:SER:O	2.24	0.51
1:C:1861:TYR:OH	1:C:1885:GLU:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2076:ALA:HB3	1:D:2077:PRO:HD3	1.91	0.51
1:A:1831:SER:HA	1:A:1936:ILE:HD12	1.93	0.51
1:B:1883:ILE:CD1	1:B:1892:MET:HE3	2.33	0.50
1:A:2099:VAL:HG22	1:A:2157:TRP:CZ2	2.46	0.50
1:C:2411:VAL:HG21	1:D:2422:ASN:HD22	1.75	0.50
1:A:2099:VAL:CG2	1:A:2157:TRP:CE2	2.95	0.50
1:D:1965:LEU:O	1:D:1969:LEU:HG	2.11	0.50
1:A:1980:LEU:HD22	1:B:2163:GLY:HA2	1.94	0.50
1:C:1788:VAL:HG23	1:C:1823:PRO:HB2	1.93	0.50
1:A:2269:ASP:O	1:A:2273:LYS:CB	2.60	0.50
1:D:1872:ILE:HG23	1:D:1877:SER:HB2	1.93	0.50
1:B:2106:VAL:CG1	1:B:2122:ILE:HB	2.42	0.50
1:A:2021:VAL:HB	1:A:2093:PRO:HG2	1.92	0.50
1:B:2237:ILE:HG22	1:B:2238:LYS:HG2	1.93	0.50
1:A:2407:LYS:O	1:A:2411:VAL:HG23	2.12	0.50
1:A:1922:TYR:CE2	1:A:1947:GLN:HG3	2.47	0.50
1:C:1986:MET:CE	1:D:2167:MET:HE3	2.42	0.50
1:C:2352:HIS:C	1:C:2352:HIS:ND1	2.65	0.49
1:C:2248:MET:HE1	1:C:2283:GLU:HA	1.94	0.49
1:B:2398:THR:CB	1:B:2402:ASN:CB	2.90	0.49
1:B:1928:ILE:HG22	1:B:1929:SER:N	2.27	0.49
1:B:2384:TRP:CE3	1:B:2385:LEU:HD23	2.47	0.49
1:D:2292:GLN:O	1:D:2295:VAL:HG22	2.11	0.49
1:B:2029:PRO:O	1:B:2323:ARG:NH1	2.46	0.49
1:D:1946:GLY:O	1:D:1948:ARG:N	2.46	0.49
1:D:2353:VAL:O	1:D:2357:SER:HB3	2.13	0.49
1:B:1791:ILE:CD1	1:B:1810:TYR:HA	2.43	0.49
1:B:2207:ILE:HG12	1:B:2207:ILE:O	2.13	0.49
1:B:1949:VAL:CG1	1:B:1991:VAL:O	2.60	0.49
1:A:2067:ASP:OD1	1:A:2323:ARG:NH2	2.46	0.49
1:B:2343:ILE:CG2	1:B:2403:ILE:CD1	2.89	0.49
1:C:2283:GLU:O	1:C:2287:LEU:HB2	2.13	0.49
1:A:2205:VAL:HG11	1:B:1938:ILE:HD13	1.94	0.49
1:B:2218:MET:HE3	1:B:2312:VAL:O	2.13	0.49
1:B:2094:VAL:HG22	1:B:2095:GLY:O	2.13	0.49
1:A:2030:ILE:HD12	1:A:2031:ASP:N	2.28	0.48
1:C:1943:VAL:HG13	1:C:1949:VAL:HG22	1.94	0.48
1:C:2370:VAL:HG23	1:C:2371:LYS:HD3	1.95	0.48
1:C:2251:ILE:HD13	1:D:1847:VAL:HG23	1.95	0.48
1:C:2340:LYS:CG	1:C:2355:ILE:HG22	2.42	0.48
1:A:1770:MET:CE	1:A:1791:ILE:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1700:ASP:O	1:B:1704:ALA:HB3	2.12	0.48
1:C:1850:VAL:CG1	1:C:1857:LYS:CB	2.91	0.48
1:A:1779:THR:HG21	1:A:1786:ARG:HD2	1.94	0.48
1:A:2388:HIS:CB	1:A:2399:ILE:HG22	2.44	0.48
1:B:2374:LEU:HD23	1:B:2380:VAL:HG21	1.96	0.48
1:C:1750:LEU:HG	1:C:1809:LEU:HD12	1.96	0.48
1:B:2199:LEU:HD23	1:B:2204:TRP:CE3	2.48	0.48
1:C:2307:MET:HG2	1:D:1905:VAL:HG11	1.94	0.48
1:B:1756:LEU:HG	1:B:1812:ARG:HB3	1.96	0.48
1:C:2298:ALA:HA	1:D:1837:MET:CE	2.44	0.48
1:B:1750:LEU:HD13	1:B:1808:LEU:HD23	1.95	0.48
1:A:1930:LEU:HD12	1:A:1950:ILE:O	2.14	0.48
1:A:2079:ALA:HB3	1:A:2136:LYS:HD3	1.96	0.48
1:A:1697:VAL:O	1:A:1701:LEU:N	2.46	0.48
1:C:2292:GLN:O	1:C:2295:VAL:HG22	2.13	0.48
1:D:2217:GLU:OE2	1:D:2333:LEU:HD11	2.14	0.48
1:C:1823:PRO:CB	1:C:1926:VAL:HG13	2.44	0.47
1:C:2339:VAL:HA	1:C:2343:ILE:HD12	1.96	0.47
1:B:2258:LEU:HB2	1:B:2279:LEU:HD13	1.95	0.47
1:D:1757:VAL:HG23	1:D:1759:MET:CE	2.44	0.47
1:B:2099:VAL:HG22	1:B:2157:TRP:CE2	2.49	0.47
1:A:2194:PRO:HD2	1:A:2197:ALA:HB3	1.97	0.47
1:B:1795:ILE:HD13	1:B:1829:ALA:HB1	1.95	0.47
1:B:1702:LEU:HD21	1:B:1706:ARG:NH2	2.29	0.47
1:D:2155:ALA:HB1	1:D:2199:LEU:HD13	1.96	0.47
1:D:2290:TYR:HA	1:D:2293:VAL:HG12	1.95	0.47
1:D:2199:LEU:HD23	1:D:2204:TRP:CE3	2.49	0.47
1:D:1707:PHE:O	1:D:1711:THR:HG23	2.15	0.47
1:C:1964:ALA:O	1:C:1968:VAL:HG13	2.14	0.47
1:B:2021:VAL:HG11	1:B:2150:PRO:HD3	1.96	0.47
1:C:2229:LEU:HD11	1:C:2237:ILE:HD12	1.95	0.47
1:C:1926:VAL:HG21	1:C:2013:MET:HE1	1.96	0.47
1:C:1862:LEU:HD21	1:D:2293:VAL:CG2	2.43	0.47
1:A:1717:ILE:CG1	1:A:1771:VAL:HG22	2.45	0.47
1:D:1950:ILE:HD13	1:D:2005:THR:HB	1.97	0.47
1:C:1835:ILE:HG22	1:D:2228:VAL:CG1	2.40	0.47
1:D:2193:ILE:CG2	1:D:2224:SER:HB2	2.45	0.47
1:A:2411:VAL:HG21	1:B:2422:ASN:HD22	1.80	0.47
1:C:2264:GLU:CB	1:C:2265:PRO:HD3	2.45	0.47
1:A:1905:VAL:HG11	1:B:2312:VAL:HG21	1.97	0.47
1:B:2373:TYR:CZ	1:B:2374:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2030:ILE:HD12	1:A:2030:ILE:C	2.35	0.46
1:D:2384:TRP:CD1	1:D:2388:HIS:CE1	3.03	0.46
1:B:2344:LEU:HD23	1:B:2355:ILE:HG12	1.96	0.46
1:C:1717:ILE:HG12	1:C:1771:VAL:HG22	1.97	0.46
1:C:1770:MET:O	1:C:1809:LEU:HD22	2.15	0.46
1:D:2332:ARG:HH21	1:D:2381:VAL:HG21	1.80	0.46
1:C:1986:MET:HE1	1:D:2167:MET:HE3	1.97	0.46
1:A:2378:ASN:O	1:A:2382:VAL:HG23	2.16	0.46
1:D:1743:LEU:HD13	1:D:1777:PHE:HB3	1.97	0.46
1:B:1922:TYR:CE2	1:B:1947:GLN:HG3	2.50	0.46
1:C:2248:MET:HE1	1:C:2283:GLU:HG3	1.97	0.46
1:B:1756:LEU:HD21	1:B:1809:LEU:HD12	1.98	0.46
1:C:2037:LEU:HD21	1:C:2320:LYS:HD3	1.98	0.46
1:A:2339:VAL:CG1	1:A:2399:ILE:HD11	2.45	0.46
1:D:2012:TYR:O	1:D:2149:LEU:HD21	2.16	0.46
1:D:2021:VAL:HG11	1:D:2150:PRO:HD3	1.97	0.46
1:B:2193:ILE:HG22	1:B:2197:ALA:HB3	1.98	0.46
1:C:2163:GLY:O	1:C:2164:MET:C	2.54	0.46
1:C:2396:ARG:O	1:C:2401:GLU:N	2.48	0.46
1:D:1875:LEU:HD13	1:D:1899:LYS:HD3	1.97	0.46
1:C:2209:ALA:H	1:C:2218:MET:HE2	1.81	0.46
1:A:2415:ILE:HG23	1:B:2415:ILE:CD1	2.45	0.45
1:D:2345:GLN:HE22	1:D:2349:GLU:CA	2.29	0.45
1:B:2045:PRO:O	1:B:2048:MET:HG2	2.16	0.45
1:C:2030:ILE:HD11	1:C:2031:ASP:OD1	2.16	0.45
1:A:2399:ILE:HG23	1:A:2400:ARG:N	2.31	0.45
1:C:2231:PRO:O	1:C:2235:VAL:HG23	2.16	0.45
1:A:2106:VAL:HG13	1:A:2122:ILE:HB	1.98	0.45
1:D:2290:TYR:O	1:D:2293:VAL:HG12	2.16	0.45
1:C:1835:ILE:HD11	1:D:2237:ILE:CG2	2.45	0.45
1:D:2048:MET:CE	1:D:2049:LEU:HD12	2.47	0.45
1:A:2232:GLU:HG2	2:A:1:RCP:C5	2.46	0.45
1:A:2236:GLU:HG2	2:A:1:RCP:H9	1.97	0.45
1:A:2353:VAL:HG13	1:A:2354:HIS:N	2.31	0.45
1:B:2076:ALA:HB3	1:B:2077:PRO:HD3	1.98	0.45
1:D:1883:ILE:HG23	1:D:1890:ARG:HB2	1.99	0.45
1:B:2099:VAL:HG11	1:B:2156:ASN:O	2.17	0.45
1:A:2241:LYS:O	1:A:2245:ILE:HG23	2.16	0.45
1:C:1993:HIS:HD2	1:C:2074:ILE:HD12	1.82	0.45
1:D:2198:GLU:OE1	1:D:2200:ARG:NH1	2.50	0.45
1:A:2092:ILE:HD11	1:A:2331:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1936:ILE:HG23	1:C:1958:ILE:HG13	1.99	0.45
1:A:2167:MET:HE2	1:B:1958:ILE:HA	1.99	0.45
1:D:2191:ILE:HG21	1:D:2207:ILE:HD11	1.97	0.45
1:D:2345:GLN:HE22	1:D:2349:GLU:C	2.21	0.45
1:A:2225:ARG:NH1	1:A:2303:THR:HG22	2.32	0.45
1:D:2191:ILE:HG21	1:D:2207:ILE:CD1	2.46	0.45
1:A:2008:GLU:O	1:A:2011:SER:HB3	2.17	0.45
1:B:2262:LEU:HD21	1:B:2275:LEU:HB2	2.00	0.44
1:B:1872:ILE:HG23	1:B:1877:SER:HB3	1.99	0.44
1:C:1786:ARG:CB	1:C:2015:LYS:HG3	2.47	0.44
1:D:2332:ARG:NH2	1:D:2375:TRP:O	2.50	0.44
1:C:2432:TYR:HE2	1:D:2416:ARG:CB	2.31	0.44
1:B:2292:GLN:O	1:B:2295:VAL:HG22	2.17	0.44
1:B:1844:MET:HB2	1:B:1844:MET:HE3	1.85	0.44
1:A:2239:PHE:CD1	1:B:1842:LYS:HE3	2.53	0.44
1:C:1818:ARG:CZ	1:C:1920:LEU:HD23	2.48	0.44
1:A:1766:ASN:N	1:A:1766:ASN:OD1	2.50	0.44
1:D:2095:GLY:O	1:D:2151:LEU:HD12	2.18	0.44
1:C:1718:TYR:CE1	1:C:1771:VAL:HG11	2.52	0.44
1:C:1863:TYR:CD2	1:C:1890:ARG:HG2	2.52	0.44
1:D:1931:VAL:HG21	1:D:1957:ILE:CD1	2.45	0.44
1:C:1986:MET:HE1	1:D:2167:MET:HE1	2.00	0.44
1:C:1987:HIS:NE2	1:C:1995:THR:HG22	2.33	0.44
1:A:2110:ALA:HB2	1:A:2118:GLU:HA	1.99	0.44
1:A:1835:ILE:HG22	1:B:2228:VAL:CG1	2.42	0.43
1:D:1918:SER:OG	1:D:1942:LEU:HD22	2.18	0.43
1:D:1971:ARG:O	1:D:1973:VAL:HG23	2.17	0.43
1:A:2306:ARG:HA	1:B:1897:ILE:HD12	2.00	0.43
1:A:1770:MET:HE1	1:A:1791:ILE:HG22	1.99	0.43
1:D:2153:ILE:HB	1:D:2191:ILE:HG23	2.01	0.43
1:D:1825:ILE:HG21	1:D:2006:ILE:HD13	2.00	0.43
1:D:2204:TRP:O	1:D:2207:ILE:HG22	2.19	0.43
1:C:2016:ASP:OD2	1:C:2018:HIS:ND1	2.52	0.43
1:D:1723:MET:HE1	1:D:2003:VAL:CG2	2.49	0.43
1:A:1985:ILE:HD11	1:B:2164:MET:HE3	1.99	0.43
1:D:2331:ARG:HD3	1:D:2382:VAL:HG11	1.98	0.43
1:D:2271:ASP:O	1:D:2275:LEU:HD12	2.17	0.43
1:B:1923:GLU:OE1	1:B:2146:ARG:NH1	2.50	0.43
1:D:1872:ILE:CG2	1:D:1877:SER:HB2	2.48	0.43
1:C:2014:PRO:HB2	1:C:2016:ASP:O	2.18	0.43
1:C:1975:THR:N	1:C:1979:GLN:OE1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1959:LEU:HD13	1:D:2160:PHE:HB2	2.01	0.43
1:A:1698:THR:HG23	1:A:1702:LEU:HD23	2.00	0.43
1:A:1840:GLU:HG3	1:A:1841:ILE:N	2.34	0.43
1:C:2430:VAL:HG23	1:C:2431:ILE:N	2.33	0.43
1:C:2217:GLU:OE2	1:C:2333:LEU:HD21	2.18	0.43
1:A:1968:VAL:HG12	2:B:2:RCP:C6	2.49	0.43
1:C:2289:ILE:HD13	1:D:1856:HIS:ND1	2.34	0.43
1:D:1922:TYR:CZ	1:D:2146:ARG:HD3	2.53	0.43
1:D:2081:THR:CG2	1:D:2128:VAL:O	2.60	0.43
1:D:2153:ILE:HD12	1:D:2191:ILE:HD12	1.98	0.43
1:D:1958:ILE:HD12	1:D:1961:GLY:HA2	2.01	0.43
1:A:1749:VAL:O	1:A:1757:VAL:HG22	2.19	0.43
1:B:2248:MET:HE3	1:B:2255:TYR:CE2	2.53	0.43
1:B:2235:VAL:HG21	1:B:2295:VAL:HA	2.01	0.43
1:D:1864:LEU:CD2	1:D:1893:ILE:HD11	2.48	0.43
1:A:2433:LEU:CD2	1:B:2419:VAL:HG21	2.49	0.43
1:C:2425:VAL:HG12	1:C:2429:CYS:HB2	2.01	0.43
1:A:2298:ALA:HA	1:B:1837:MET:CE	2.49	0.42
1:B:2003:VAL:HA	1:B:2006:ILE:HD12	2.01	0.42
2:C:3:RCP:H25	2:C:3:RCP:H292	1.74	0.42
1:A:1723:MET:HE2	1:A:1723:MET:HB3	1.81	0.42
1:C:2030:ILE:CD1	1:C:2031:ASP:OD1	2.67	0.42
1:B:2308:LEU:CD1	1:B:2316:ILE:HG23	2.34	0.42
1:D:2331:ARG:CZ	1:D:2386:GLU:OE2	2.68	0.42
1:A:1743:LEU:HD13	1:A:1777:PHE:HB3	2.02	0.42
1:D:1926:VAL:CG2	1:D:2013:MET:CE	2.93	0.42
1:C:1845:PHE:CE1	1:C:1862:LEU:HD22	2.54	0.42
1:D:2407:LYS:O	1:D:2411:VAL:HG23	2.20	0.42
1:D:2094:VAL:HG21	1:D:2152:MET:HG3	2.01	0.42
1:C:2306:ARG:HA	1:D:1897:ILE:HD12	2.01	0.42
1:C:2316:ILE:O	1:C:2317:LEU:HD23	2.19	0.42
1:C:1789:ILE:HD12	1:C:1817:ALA:CB	2.46	0.42
1:D:1756:LEU:HG	1:D:1812:ARG:HB3	2.01	0.42
1:A:1756:LEU:HD21	1:A:1809:LEU:CD1	2.49	0.42
1:B:2361:ARG:O	1:B:2364:VAL:HG22	2.19	0.42
1:D:2252:ASP:OD2	1:D:2286:LEU:HD11	2.19	0.42
1:D:1700:ASP:O	1:D:1704:ALA:HB3	2.19	0.42
1:B:1739:PRO:HD2	1:B:1742:ILE:HD12	2.02	0.42
1:D:1926:VAL:HG13	1:D:2013:MET:HE1	2.01	0.42
1:B:2245:ILE:HD12	1:B:2283:GLU:OE1	2.19	0.42
1:A:2419:VAL:CG1	1:A:2426:ALA:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2339:VAL:O	1:C:2343:ILE:HB	2.19	0.42
1:D:1772:ALA:HA	1:D:1790:VAL:O	2.19	0.42
1:C:2142:LYS:O	1:C:2146:ARG:HD3	2.19	0.42
1:D:1757:VAL:HG23	1:D:1759:MET:HE3	2.02	0.42
1:A:1811:LEU:HD22	1:A:1913:MET:SD	2.60	0.42
1:A:2110:ALA:HB2	1:A:2119:ALA:N	2.34	0.42
1:B:2110:ALA:HB2	1:B:2119:ALA:N	2.35	0.42
1:D:2345:GLN:NE2	1:D:2345:GLN:O	2.52	0.42
1:A:2361:ARG:O	1:A:2365:GLU:HB2	2.20	0.42
1:C:2094:VAL:HG22	1:C:2095:GLY:O	2.20	0.42
1:A:2425:VAL:HG13	1:B:2412:LEU:HD21	2.02	0.42
1:B:2044:ASP:HB3	1:B:2047:TRP:CD2	2.54	0.42
1:B:2438:SER:O	1:B:2442:ARG:N	2.53	0.42
1:D:2042:PRO:HB3	1:D:2101:THR:O	2.19	0.41
1:B:2278:ARG:O	1:B:2281:ALA:HB3	2.20	0.41
1:A:2343:ILE:HG21	1:A:2403:ILE:HG21	1.93	0.41
1:D:2191:ILE:CG2	1:D:2207:ILE:HD11	2.50	0.41
1:B:2048:MET:HE1	1:B:2154:PHE:CD2	2.55	0.41
1:C:1960:THR:HG21	2:D:4:RCP:H20	2.01	0.41
1:C:2205:VAL:HG11	1:D:1938:ILE:HD13	2.02	0.41
1:D:1717:ILE:HG12	1:D:1771:VAL:HG22	2.02	0.41
1:B:2352:HIS:HA	1:B:2355:ILE:HD12	2.02	0.41
1:D:1844:MET:CE	1:D:1864:LEU:HD13	2.50	0.41
1:D:1864:LEU:HD21	1:D:1893:ILE:HD11	2.02	0.41
1:A:2141:ILE:HD13	1:A:2182:LEU:HD21	2.02	0.41
1:B:1883:ILE:CD1	1:B:1892:MET:CE	2.96	0.41
1:C:1702:LEU:HD21	1:C:1706:ARG:HH11	1.84	0.41
1:C:2012:TYR:O	1:C:2149:LEU:HD21	2.20	0.41
1:D:1926:VAL:CG1	1:D:2013:MET:HE2	2.51	0.41
1:B:2094:VAL:HG21	1:B:2152:MET:CG	2.49	0.41
1:D:1987:HIS:O	1:D:2077:PRO:HG2	2.21	0.41
1:A:1905:VAL:CG1	1:B:2312:VAL:HG21	2.50	0.41
1:B:2012:TYR:O	1:B:2149:LEU:HD21	2.21	0.41
1:B:1985:ILE:HG22	1:B:1986:MET:HE2	2.03	0.41
1:C:1698:THR:HA	1:C:1702:LEU:CB	2.49	0.41
1:B:1700:ASP:O	1:B:1704:ALA:CB	2.68	0.41
1:A:1911:SER:HB3	1:A:1938:ILE:HD13	2.01	0.41
1:B:2198:GLU:HA	1:B:2225:ARG:O	2.20	0.41
1:B:1943:VAL:CG1	1:B:1949:VAL:HG21	2.51	0.41
1:A:2387:GLN:NE2	1:A:2398:THR:HG21	2.34	0.41
1:D:1804:PRO:HD3	1:D:1907:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2219:TYR:HB3	1:D:2317:LEU:HD12	2.02	0.41
1:C:2045:PRO:HG2	1:C:2083:VAL:HG21	2.03	0.41
1:B:2264:GLU:N	1:B:2265:PRO:HD3	2.36	0.41
1:D:1949:VAL:HG13	1:D:1992:SER:HA	2.03	0.41
1:A:2339:VAL:HG11	1:A:2399:ILE:HD11	2.03	0.41
1:D:1743:LEU:HD12	1:D:1744:THR:N	2.36	0.41
1:A:2229:LEU:HD12	1:B:1835:ILE:HD12	2.03	0.41
1:A:2054:HIS:CD2	1:A:2057:LEU:HB2	2.56	0.41
1:B:2073:GLU:OE2	1:B:2083:VAL:HG13	2.21	0.41
1:B:2023:ILE:HD13	1:B:2092:ILE:HG12	2.03	0.41
1:A:2172:LEU:HA	1:A:2172:LEU:HD12	1.94	0.41
1:D:1723:MET:HE2	1:D:1723:MET:HB3	1.94	0.41
1:D:1926:VAL:HG22	1:D:2013:MET:CE	2.50	0.41
1:C:1793:ASN:ND2	1:C:1830:ASN:HD22	2.19	0.41
1:A:1748:LEU:HB3	1:A:1756:LEU:HD22	2.03	0.41
1:C:2205:VAL:CG1	1:D:1938:ILE:HD13	2.51	0.41
1:A:1775:MET:HB3	1:A:1775:MET:HE2	1.90	0.41
1:A:2438:SER:O	1:A:2442:ARG:N	2.49	0.41
1:D:1931:VAL:HG22	1:D:1943:VAL:HG21	2.02	0.40
1:B:2079:ALA:HB3	1:B:2136:LYS:HD3	2.02	0.40
1:B:2185:TYR:CB	1:B:2189:ILE:HD11	2.52	0.40
1:B:1720:PHE:N	1:B:1721:PRO:CD	2.85	0.40
1:B:1880:CYS:HA	1:B:1894:THR:HG23	2.02	0.40
1:D:2088:ARG:HA	1:D:2092:ILE:O	2.20	0.40
1:D:1818:ARG:HD3	1:D:1921:ALA:HA	2.03	0.40
1:A:1816:MET:O	1:A:1819:ALA:HB3	2.21	0.40
1:C:2126:GLY:O	1:C:2128:VAL:HG23	2.21	0.40
1:C:2287:LEU:N	1:C:2288:PRO:CD	2.85	0.40
1:D:1707:PHE:HB3	3:D:12:HOH:O	2.21	0.40
1:D:1702:LEU:HD21	1:D:1706:ARG:NH2	2.37	0.40
1:D:1723:MET:HE1	1:D:2003:VAL:HG23	2.03	0.40
1:B:2099:VAL:HG22	1:B:2157:TRP:CZ2	2.56	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	746/760 (98%)	693 (93%)	50 (7%)	3 (0%)	39	80
1	B	744/760 (98%)	691 (93%)	49 (7%)	4 (0%)	34	78
1	C	734/760 (97%)	684 (93%)	45 (6%)	5 (1%)	26	72
1	D	729/760 (96%)	682 (94%)	38 (5%)	9 (1%)	16	60
All	All	2953/3040 (97%)	2750 (93%)	182 (6%)	21 (1%)	26	72

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1735	PRO
1	C	1947	GLN
1	D	2349	GLU
1	D	2355	ILE
1	B	2265	PRO
1	D	1947	GLN
1	D	2351	SER
1	A	2398	THR
1	A	2438	SER
1	B	1740	LYS
1	B	2347	SER
1	C	2264	GLU
1	D	1904	GLY
1	D	2341	GLN
1	B	1799	ILE
1	C	1799	ILE
1	D	1799	ILE
1	D	2288	PRO
1	D	2348	GLY
1	A	1799	ILE
1	C	2439	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	558/650 (86%)	553 (99%)	5 (1%)	84	95
1	B	578/650 (89%)	572 (99%)	6 (1%)	82	95
1	C	576/650 (89%)	572 (99%)	4 (1%)	88	97
1	D	568/650 (87%)	563 (99%)	5 (1%)	84	95
All	All	2280/2600 (88%)	2260 (99%)	20 (1%)	84	95

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2108	VAL
1	A	2239	PHE
1	A	2242	LYS
1	A	2324	THR
1	A	2331	ARG
1	B	1874	SER
1	B	2039	SER
1	B	2135	TYR
1	B	2146	ARG
1	B	2239	PHE
1	B	2315	ASP
1	C	2039	SER
1	C	2135	TYR
1	C	2239	PHE
1	C	2432	TYR
1	D	1864	LEU
1	D	1960	THR
1	D	2129	TRP
1	D	2146	ARG
1	D	2239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1793	ASN
1	A	1993	HIS
1	A	2054	HIS
1	A	2387	GLN
1	A	2408	HIS
1	A	2422	ASN

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Mol	Chain	Res	Type
1	B	2139	GLN
1	B	2170	GLN
1	B	2184	GLN
1	B	2352	HIS
1	B	2422	ASN
1	C	1780	GLN
1	C	1793	ASN
1	C	1879	HIS
1	C	1966	ASN
1	C	1993	HIS
1	C	2127	GLN
1	C	2187	GLN
1	D	2123	GLN
1	D	2127	GLN
1	D	2345	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	RCP	A	1	-	41,41,41	1.29	5 (12%)	58,58,58	1.68	12 (20%)
2	RCP	B	2	-	41,41,41	1.32	5 (12%)	58,58,58	1.84	12 (20%)
2	RCP	C	3	-	41,41,41	1.21	4 (9%)	58,58,58	1.52	10 (17%)
2	RCP	D	4	-	41,41,41	1.25	4 (9%)	58,58,58	1.62	12 (20%)

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	RCP	A	1	-	-	0/20/48/48	0/6/6/6
2	RCP	B	2	-	-	0/20/48/48	0/6/6/6
2	RCP	C	3	-	-	0/20/48/48	0/6/6/6
2	RCP	D	4	-	-	0/20/48/48	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	RCP	C14-C15	-3.96	1.46	1.50
2	B	2	RCP	C14-C15	-3.83	1.46	1.50
2	D	4	RCP	C14-C15	-3.54	1.46	1.50
2	C	3	RCP	C14-C15	-2.78	1.47	1.50
2	A	1	RCP	C1-C6	-2.69	1.37	1.42
2	A	1	RCP	C13-C8	-2.61	1.38	1.42
2	B	2	RCP	C13-C8	-2.49	1.38	1.42
2	C	3	RCP	C1-C6	-2.40	1.38	1.42
2	D	4	RCP	C13-C8	-2.34	1.38	1.42
2	C	3	RCP	C13-C8	-2.33	1.38	1.42
2	D	4	RCP	C1-C6	-2.30	1.38	1.42
2	B	2	RCP	C1-C6	-2.27	1.38	1.42
2	B	2	RCP	C14-C13	-2.07	1.38	1.41
2	A	1	RCP	C18-N15	-2.06	1.43	1.47
2	A	1	RCP	C26-N26	2.33	1.38	1.34
2	C	3	RCP	C26-N26	2.44	1.38	1.34
2	D	4	RCP	C26-N26	2.58	1.38	1.34
2	B	2	RCP	C26-N26	2.84	1.39	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	RCP	C25-C26-N26	-7.00	112.44	119.06
2	B	2	RCP	C25-C26-N26	-6.43	112.98	119.06
2	C	3	RCP	O15-C15-C14	-5.23	116.44	121.64
2	B	2	RCP	O15-C15-C14	-4.80	116.86	121.64
2	D	4	RCP	O15-C15-C14	-4.27	117.39	121.64
2	D	4	RCP	C25-C26-N26	-3.60	115.65	119.06
2	A	1	RCP	O15-C15-C14	-3.58	118.08	121.64
2	B	2	RCP	C23-C22-C21	-3.25	106.63	110.97
2	C	3	RCP	C18-C19-C20	-3.22	105.90	110.80
2	C	3	RCP	C22-C21-N20	-3.13	105.77	111.15
2	D	4	RCP	C23-C22-C21	-3.09	106.84	110.97
2	D	4	RCP	C22-C21-N20	-2.92	106.14	111.15
2	C	3	RCP	C25-C26-N26	-2.90	116.32	119.06
2	A	1	RCP	O28-C28-C27	-2.63	105.80	111.84
2	D	4	RCP	C18-C19-C20	-2.58	106.89	110.80
2	B	2	RCP	O28-C28-C27	-2.54	106.01	111.84
2	A	1	RCP	C18-C19-C20	-2.53	106.96	110.80
2	A	1	RCP	C14-C15-N15	-2.49	115.21	117.75
2	B	2	RCP	C29-N26-C26	-2.31	114.72	123.19
2	D	4	RCP	C29-N26-C26	-2.30	114.77	123.19
2	A	1	RCP	C19-C18-N15	-2.26	107.79	111.07
2	C	3	RCP	C9-C8-C7	-2.14	118.36	121.99
2	B	2	RCP	C23-C25-C26	-2.12	105.73	109.69
2	A	1	RCP	C23-C22-C21	-2.03	108.26	110.97
2	C	3	RCP	O28-C30-C29	-2.01	107.22	111.84
2	D	4	RCP	C21-N20-C24	2.06	109.90	108.09
2	B	2	RCP	C27-N26-C29	2.12	116.50	112.56
2	D	4	RCP	C23-C25-C24	2.21	114.16	109.72
2	D	4	RCP	C30-C29-N26	2.23	114.68	109.90
2	C	3	RCP	C16-N15-C18	2.26	116.74	112.56
2	B	2	RCP	O15-C15-N15	2.30	126.08	122.42
2	A	1	RCP	C23-C25-C24	2.62	114.98	109.72
2	A	1	RCP	O26-C26-N26	2.66	124.98	121.66
2	A	1	RCP	O15-C15-N15	2.70	126.72	122.42
2	A	1	RCP	C16-N15-C18	2.72	117.61	112.56
2	C	3	RCP	C25-C24-N20	2.76	114.36	110.81
2	A	1	RCP	C27-N26-C29	2.80	117.75	112.56
2	B	2	RCP	O26-C26-N26	2.86	125.24	121.66
2	D	4	RCP	C28-C27-N26	2.94	116.20	109.90
2	C	3	RCP	C23-C25-C24	3.00	115.74	109.72
2	C	3	RCP	C14-C15-N15	3.10	120.92	117.75
2	B	2	RCP	C23-C25-C24	3.55	116.85	109.72
2	B	2	RCP	C25-C24-N20	3.96	115.90	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	RCP	C25-C24-N20	4.07	116.03	110.81
2	D	4	RCP	C27-N26-C29	4.09	120.15	112.56
2	B	2	RCP	C21-N20-C24	4.25	111.81	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	RCP	3	0
2	B	2	RCP	2	0
2	C	3	RCP	1	0
2	D	4	RCP	1	0

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	750/760 (98%)	-0.36	17 (2%) 64 49	27, 37, 48, 62	0
1	B	748/760 (98%)	-0.44	7 (0%) 85 78	30, 37, 51, 65	0
1	C	742/760 (97%)	-0.26	20 (2%) 58 44	27, 37, 53, 62	0
1	D	733/760 (96%)	-0.40	10 (1%) 78 65	29, 36, 50, 61	0
All	All	2973/3040 (97%)	-0.37	54 (1%) 71 58	27, 37, 51, 65	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2342	GLU	4.3
1	C	1700	ASP	4.0
1	A	1883	ILE	3.4
1	B	2391	ALA	3.4
1	D	2390	GLN	3.3
1	A	1700	ASP	3.3
1	A	2263	GLY	3.2
1	D	1697	VAL	3.2
1	C	1736	ASP	3.2
1	B	2265	PRO	3.1
1	C	2443	ALA	3.1
1	C	1698	THR	3.0
1	C	2342	GLU	3.0
1	D	1698	THR	3.0
1	C	1889	SER	3.0
1	C	2397	SER	3.0
1	A	2269	ASP	2.9
1	D	2391	ALA	2.9
1	A	2262	LEU	2.8
1	B	1700	ASP	2.7
1	A	2266	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	2346	ALA	2.6
1	B	2390	GLN	2.5
1	D	2373	TYR	2.5
1	A	1752	SER	2.5
1	D	1700	ASP	2.5
1	C	2264	GLU	2.4
1	C	2347	SER	2.4
1	D	2374	LEU	2.4
1	A	2115	LEU	2.4
1	A	1887	GLY	2.4
1	C	2265	PRO	2.3
1	D	2353	VAL	2.3
1	A	2265	PRO	2.3
1	C	2372	ALA	2.3
1	A	2408	HIS	2.3
1	C	2438	SER	2.3
1	C	1760	ASN	2.3
1	A	2353	VAL	2.3
1	C	2354	HIS	2.2
1	C	2427	VAL	2.2
1	C	2445	VAL	2.1
1	A	2116	ASP	2.1
1	A	1735	PRO	2.1
1	B	2341	GLN	2.1
1	C	2115	LEU	2.1
1	C	2263	GLY	2.1
1	B	2117	SER	2.0
1	D	2056	THR	2.0
1	B	2053	PRO	2.0
1	A	1699	LYS	2.0
1	C	1885	GLU	2.0
1	A	1882	HIS	2.0
1	A	2390	GLN	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	RCP	A	1	36/36	0.93	0.21	1.39	35,36,46,47	0
2	RCP	B	2	36/36	0.95	0.22	1.00	41,46,50,51	0
2	RCP	D	4	36/36	0.93	0.22	0.69	32,35,36,37	0
2	RCP	C	3	36/36	0.95	0.19	0.24	34,37,38,39	0

6.5 Other polymers

There are no such residues in this entry.