



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:50 AM GMT

PDB ID : 2UZA
Title : CRYSTAL STRUCTURE OF THE FREE RADICAL INTERMEDIATE OF
PYRUVATE:FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIB-
RIO AFRICANUS
Authors : Chabriere, E.; Cavazza, C.; Contreras-Martel, C.; Fontecilla-Camps, J.C.
Deposited on : 2007-04-27
Resolution : 2.42 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

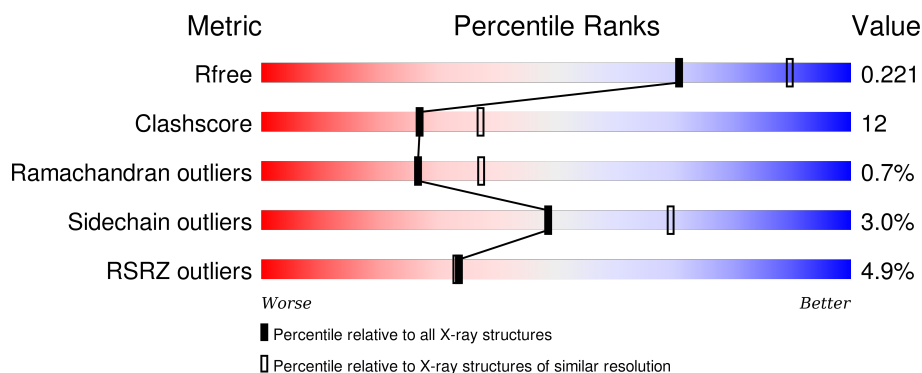
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	1231	<div> <div>7%</div> <div>73%</div> <div>25%</div> <div>•</div> </div>
1	B	1231	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>

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
5	CA	A	1239	-	-	-	X
6	CO2	A	1240	-	-	-	X
6	CO2	B	1240	-	-	-	X

2 Entry composition [i](#)

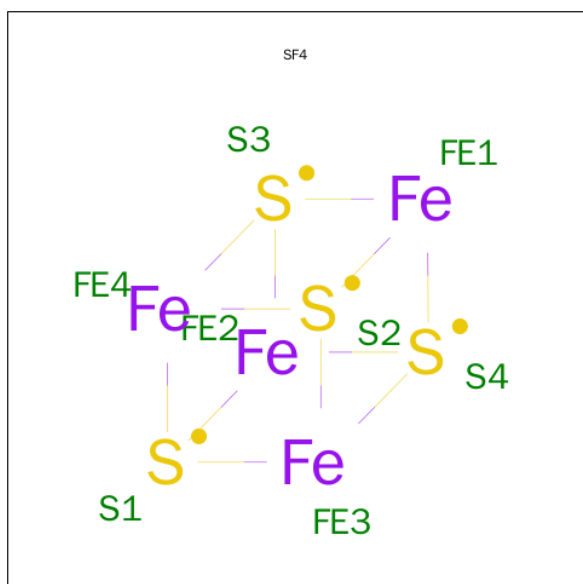
There are 7 unique types of molecules in this entry. The entry contains 19846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE FERREDONIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



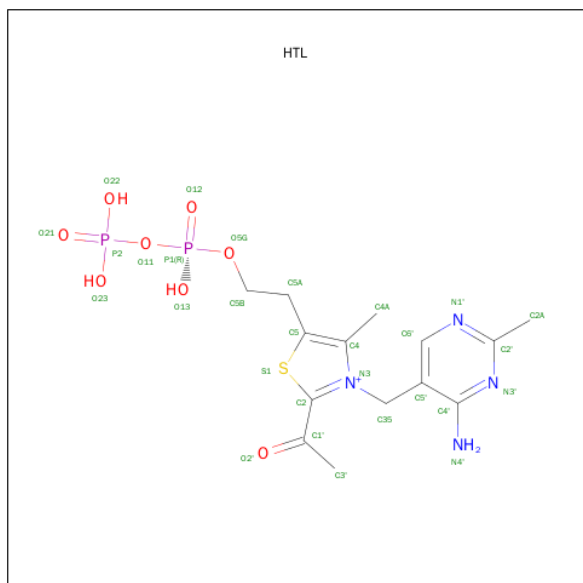
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
3	B	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0

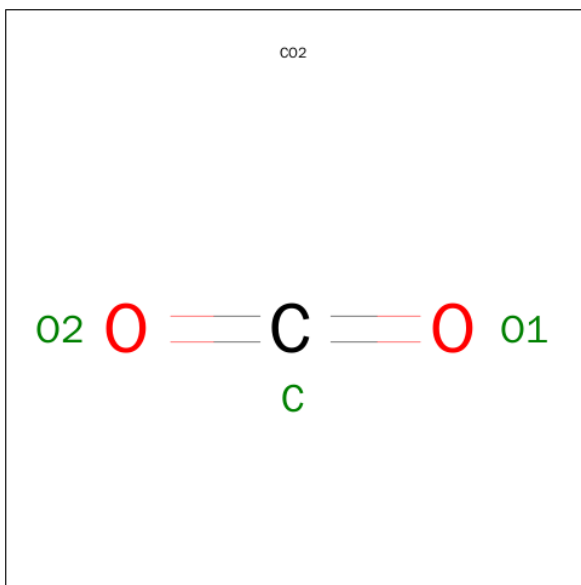
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂).



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

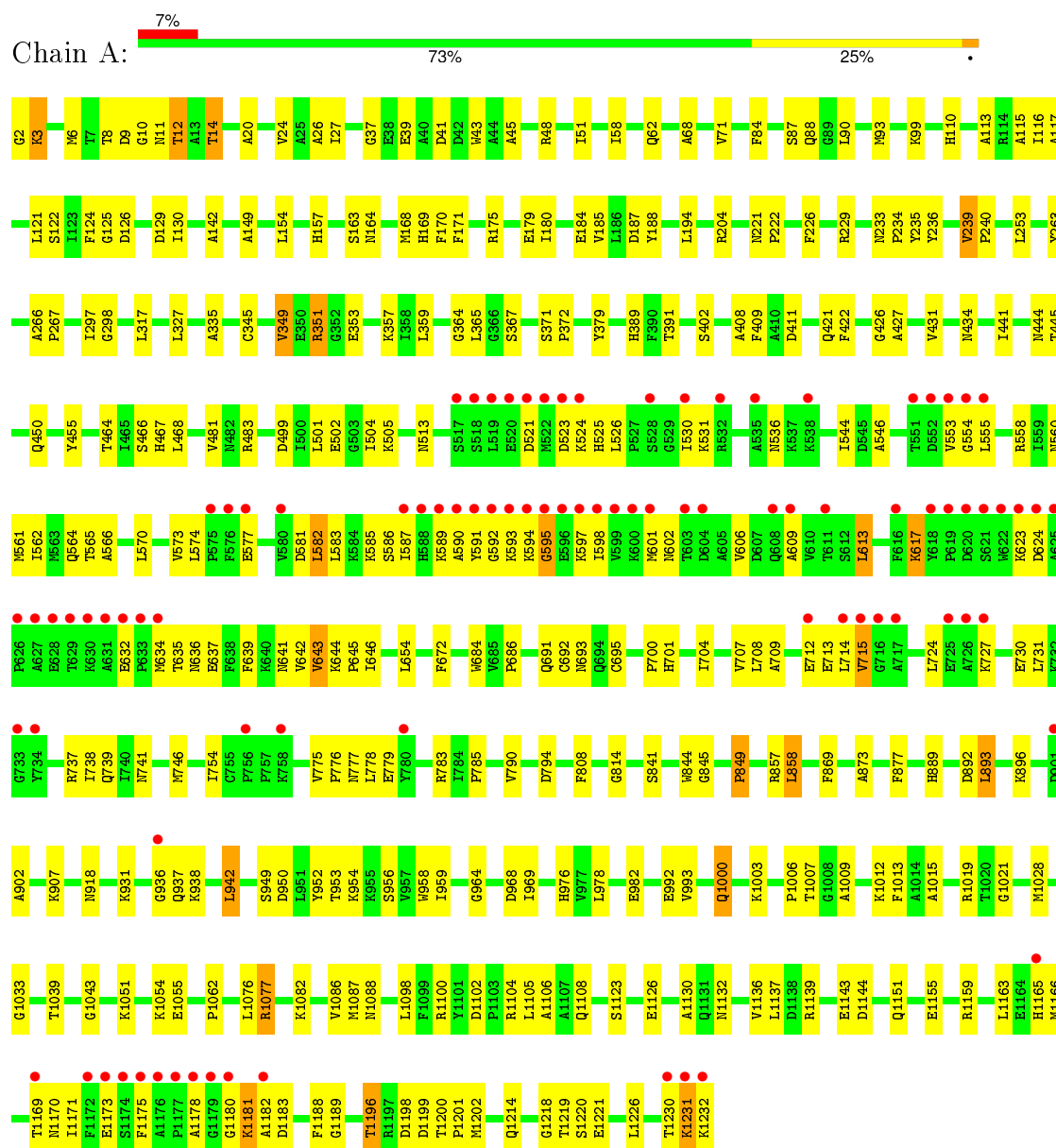
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	410	Total	O	0	0
			410	410		
7	B	554	Total	O	0	0
			554	554		

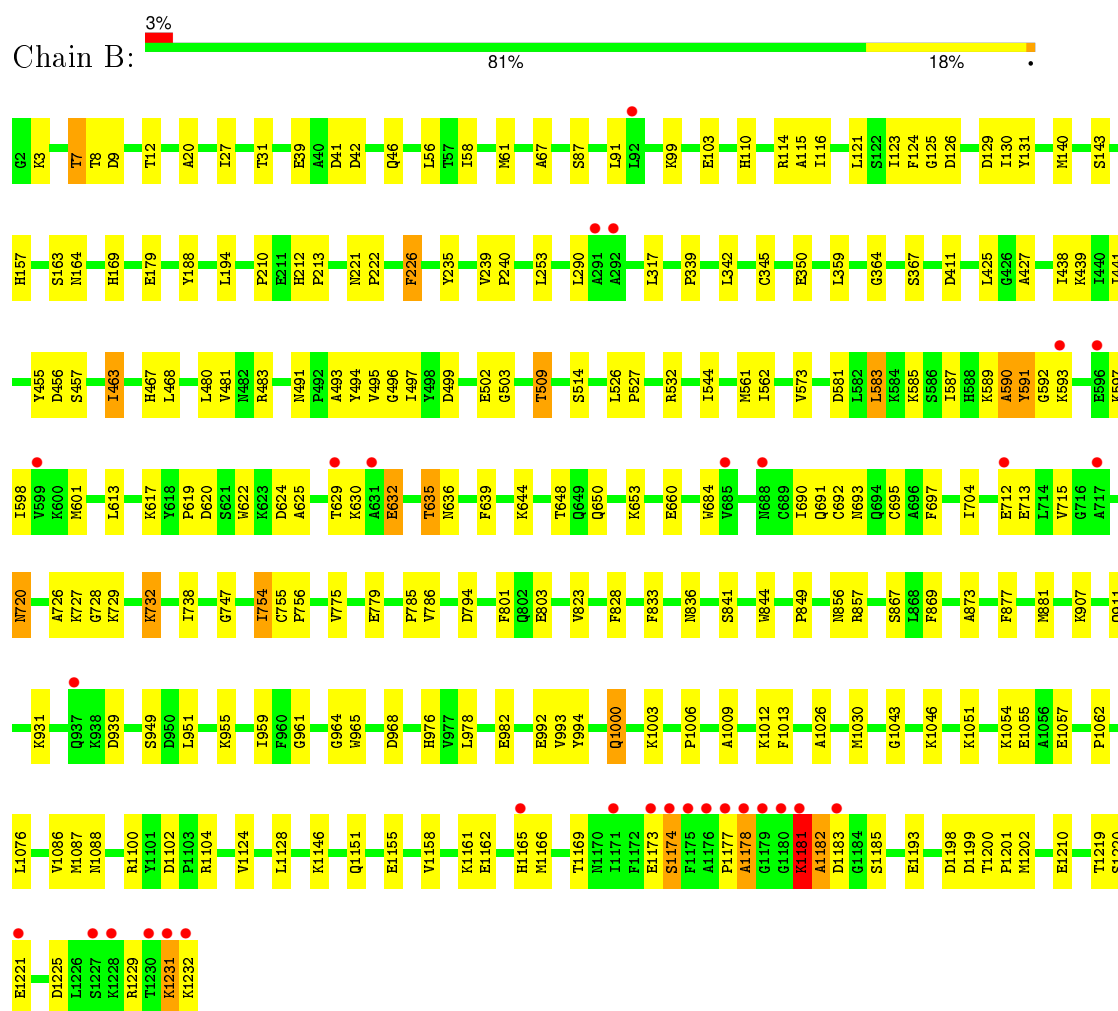
3 Residue-property plots

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: PYRUVATE FERREDOXIN OXIDOREDUCTASE



• Molecule 1: PYRUVATE FERREDOXIN OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.95Å 146.16Å 211.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 – 2.42 47.47 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.47-2.42) 99.2 (47.47-2.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.171 , 0.226 0.167 , 0.221	Depositor DCC
R_{free} test set	5121 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 101383 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19846	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: MG, CO2, CA, SF4, HTL

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	0.44	0/9585	0.67	2/12954 (0.0%)
1	B	0.45	0/9585	0.69	2/12954 (0.0%)
All	All	0.45	0/19170	0.68	4/25908 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLY	N-CA-C	6.14	128.46	113.10
1	A	125	GLY	N-CA-C	5.87	127.77	113.10
1	B	364	GLY	N-CA-C	5.37	126.52	113.10
1	A	364	GLY	N-CA-C	5.34	126.44	113.10

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	9383	0	9262	271	0
1	B	9383	0	9262	212	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0
3	A	29	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	18	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	1	0
7	A	410	0	0	7	0
7	B	554	0	0	13	0
All	All	19846	0	18560	451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1236:HTL:C2	3:B:1236:HTL:C1'	1.89	1.47
3:A:1236:HTL:C2	3:A:1236:HTL:C1'	1.94	1.45
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.43	1.00
1:A:635:THR:HG22	1:A:636:ASN:H	1.25	1.00
1:B:1200:THR:HG22	1:B:1202:MET:H	1.25	0.97
1:A:9:ASP:OD2	1:A:12:THR:HG23	1.66	0.94
1:A:1200:THR:HG22	1:A:1202:MET:H	1.31	0.94
1:B:12:THR:HG22	1:B:39:GLU:OE1	1.68	0.92
1:A:1230:THR:O	1:A:1232:LYS:HG2	1.71	0.91
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.36	0.90
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.23	0.87
1:A:526:LEU:HD11	1:A:530:ILE:HG21	1.58	0.84
1:A:593:LYS:HG3	1:A:594:LYS:H	1.41	0.84
1:B:877:PHE:HE1	1:B:982:GLU:HG3	1.43	0.84
1:B:1200:THR:HG22	1:B:1202:MET:N	1.94	0.83
1:B:493:ALA:O	1:B:497:ILE:HD13	1.79	0.82
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.46	0.81
1:B:1181:LYS:HD2	1:B:1182:ALA:H	1.46	0.80
1:A:1019:ARG:HH22	1:B:1181:LYS:HA	1.45	0.80
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.63	0.80
1:A:1219:THR:HG22	1:A:1221:GLU:H	1.46	0.79
1:A:635:THR:HG22	1:A:636:ASN:N	1.99	0.78
1:A:635:THR:HG23	1:A:672:PHE:CD2	2.20	0.77
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.29	0.77
1:A:1200:THR:HG22	1:A:1202:MET:N	1.99	0.77
1:B:9:ASP:OD2	1:B:12:THR:HG23	1.85	0.76
1:B:635:THR:CG2	1:B:639:PHE:HB3	2.16	0.76
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.68	0.76
1:B:1200:THR:CG2	1:B:1202:MET:H	1.99	0.76
1:A:1019:ARG:HH12	1:B:1181:LYS:H	1.34	0.75
1:B:877:PHE:CE1	1:B:982:GLU:HG3	2.21	0.75
1:A:1200:THR:CG2	1:A:1202:MET:H	2.00	0.73
1:A:637:GLU:HG3	1:A:641:ASN:HD21	1.54	0.73
1:A:593:LYS:HG3	1:A:594:LYS:N	2.03	0.73
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.04	0.72
1:A:992:GLU:O	1:A:993:VAL:HG13	1.90	0.71
1:B:775:VAL:O	1:B:779:GLU:HG2	1.90	0.71
1:B:635:THR:HG23	1:B:639:PHE:HB3	1.72	0.71
1:B:110:HIS:CD2	1:B:169:HIS:HD2	2.07	0.70
1:A:1019:ARG:NH2	1:B:1181:LYS:HA	2.05	0.70
1:B:691:GLN:HE22	1:B:727:LYS:H	1.39	0.70
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.74	0.70
1:A:1198:ASP:OD2	1:A:1200:THR:HB	1.92	0.69
1:B:463:ILE:HD13	1:B:494:TYR:CE1	2.27	0.69
1:A:12:THR:HG22	1:A:39:GLU:OE1	1.93	0.69
1:A:357:LYS:HE3	1:A:359:LEU:HD21	1.75	0.69
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.10	0.68
1:A:602:ASN:O	1:A:606:VAL:HG23	1.94	0.68
1:A:1180:GLY:O	1:A:1181:LYS:HB2	1.93	0.68
1:A:1003:LYS:HZ2	1:B:976:HIS:HD2	1.41	0.68
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.29	0.68
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.76	0.68
1:A:411:ASP:HB2	1:A:483:ARG:HD2	1.76	0.67
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.76	0.67
1:A:1076:LEU:HD13	1:A:1086:VAL:HG21	1.75	0.67
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.94	0.67
1:B:1198:ASP:OD2	1:B:1200:THR:HB	1.94	0.67
1:A:902:ALA:O	1:A:907:LYS:HE3	1.95	0.67
1:B:438:ILE:HD11	1:B:468:LEU:HD22	1.77	0.66
1:A:239:VAL:HG13	1:A:240:PRO:HD3	1.78	0.66
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.76	0.66
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.96	0.66
1:A:467:HIS:HD2	1:A:481:VAL:H	1.42	0.66
1:A:99:LYS:HE3	1:B:867:SER:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:THR:HG21	7:B:2265:HOH:O	1.95	0.65
1:A:1077:ARG:HG2	1:A:1130:ALA:O	1.95	0.65
1:A:1028:MET:HE3	7:B:2444:HOH:O	1.96	0.65
1:A:635:THR:HG21	1:A:639:PHE:CD2	2.31	0.65
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	1.78	0.65
1:B:467:HIS:CD2	1:B:481:VAL:H	2.15	0.65
1:A:501:LEU:O	1:A:504:ILE:HG22	1.97	0.65
1:A:737:ARG:HE	1:A:739:GLN:NE2	1.94	0.64
1:A:635:THR:HG23	1:A:672:PHE:CG	2.32	0.64
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.78	0.64
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.98	0.64
1:B:3:LYS:HE2	1:B:253:LEU:O	1.97	0.63
1:B:1151:GLN:O	1:B:1155:GLU:HG3	1.98	0.63
1:A:2:GLY:N	1:A:187:ASP:OD2	2.32	0.63
1:B:1200:THR:CG2	1:B:1202:MET:HB2	2.29	0.63
1:B:499:ASP:OD2	1:B:502:GLU:HB2	1.98	0.62
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.81	0.62
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.14	0.62
1:A:591:TYR:C	1:A:593:LYS:H	2.03	0.62
1:A:1155:GLU:HG2	1:B:1173:GLU:OE2	2.00	0.62
1:B:992:GLU:O	1:B:993:VAL:HG13	1.99	0.62
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.80	0.62
1:B:691:GLN:NE2	1:B:727:LYS:H	1.97	0.62
1:A:544:ILE:HD12	1:A:613:LEU:HD13	1.80	0.61
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.80	0.61
1:A:10:GLY:O	1:A:14:THR:HG23	2.00	0.61
1:B:907:LYS:O	1:B:911:GLN:HG3	2.00	0.61
1:A:635:THR:CG2	1:A:636:ASN:H	2.08	0.61
1:B:467:HIS:HD2	1:B:481:VAL:H	1.48	0.61
1:A:467:HIS:CD2	1:A:481:VAL:H	2.19	0.61
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.83	0.61
1:B:1200:THR:HG21	1:B:1202:MET:HB2	1.83	0.60
1:A:110:HIS:CD2	1:A:169:HIS:HD2	2.16	0.60
1:A:558:ARG:HG2	1:A:560:ASN:ND2	2.16	0.60
1:B:8:THR:HB	1:B:12:THR:OG1	2.01	0.60
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.83	0.60
1:B:598:ILE:HD13	1:B:601:MET:HE2	1.83	0.60
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.84	0.60
1:B:650:GLN:NE2	1:B:653:LYS:NZ	2.50	0.60
1:B:630:LYS:O	1:B:630:LYS:HG3	2.01	0.60
1:B:591:TYR:C	1:B:593:LYS:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.17	0.59
1:A:553:VAL:HG23	1:A:555:LEU:HG	1.84	0.59
1:B:425:LEU:HD22	1:B:491:ASN:ND2	2.17	0.59
1:A:1051:LYS:HE3	1:A:1100:ARG:NH1	2.17	0.59
1:A:554:GLY:HA3	1:A:601:MET:CE	2.32	0.59
1:A:229:ARG:HD2	7:B:2048:HOH:O	2.02	0.59
1:B:931:LYS:HD2	7:B:2430:HOH:O	2.01	0.59
1:A:593:LYS:CG	1:A:594:LYS:H	2.14	0.59
1:A:637:GLU:HG3	1:A:641:ASN:ND2	2.17	0.59
1:B:1166:MET:O	1:B:1169:THR:HG22	2.03	0.59
1:A:936:GLY:O	1:A:938:LYS:HD3	2.03	0.59
1:A:1231:LYS:HG3	1:A:1232:LYS:N	2.14	0.59
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.85	0.58
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.18	0.58
1:A:1019:ARG:HH12	1:B:1181:LYS:N	2.01	0.58
1:B:598:ILE:HD13	1:B:601:MET:CE	2.33	0.58
1:B:591:TYR:C	1:B:593:LYS:N	2.57	0.58
1:A:691:GLN:HE22	1:A:727:LYS:H	1.52	0.58
1:A:1003:LYS:HZ2	1:B:976:HIS:CD2	2.20	0.58
1:B:1000:GLN:NE2	1:B:1000:GLN:H	2.02	0.58
1:A:455:TYR:HB2	1:B:1201:PRO:HD3	1.85	0.58
1:A:345:CYS:O	1:A:349:VAL:HG13	2.04	0.57
1:B:754:ILE:HG12	7:B:2479:HOH:O	2.03	0.57
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.02	0.57
1:B:598:ILE:HA	1:B:601:MET:HE2	1.85	0.57
1:B:590:ALA:O	1:B:591:TYR:C	2.41	0.57
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.86	0.57
1:B:650:GLN:HE22	1:B:653:LYS:NZ	2.03	0.57
1:A:163:SER:O	1:A:164:ASN:HB2	2.03	0.57
1:B:1158:VAL:O	1:B:1162:GLU:HG3	2.04	0.57
1:A:3:LYS:HE2	1:A:253:LEU:O	2.05	0.57
1:B:496:GLY:C	1:B:497:ILE:HD12	2.24	0.57
1:A:1200:THR:CG2	1:A:1202:MET:HB2	2.35	0.56
1:B:497:ILE:HD12	1:B:497:ILE:N	2.20	0.56
1:A:877:PHE:HE1	1:A:982:GLU:HG3	1.70	0.56
1:B:644:LYS:O	1:B:648:THR:HG23	2.04	0.56
1:B:591:TYR:O	1:B:593:LYS:N	2.38	0.56
1:A:581:ASP:OD2	1:A:585:LYS:HE3	2.06	0.56
1:A:635:THR:HG21	1:A:639:PHE:CG	2.41	0.56
1:B:803:GLU:OE1	1:B:856:ASN:HB2	2.06	0.56
1:B:42:ASP:O	1:B:46:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:MET:HG3	1:B:67:ALA:HA	1.86	0.55
1:A:950:ASP:OD2	1:B:212:HIS:HE1	1.89	0.55
1:A:731:LEU:CD2	1:A:790:VAL:HG11	2.36	0.55
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.42	0.55
1:A:1188:PHE:HE1	1:A:1196:THR:HG23	1.70	0.55
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.03	0.55
1:A:426:GLY:O	1:A:427:ALA:HB3	2.06	0.55
1:B:1219:THR:CG2	1:B:1220:SER:N	2.70	0.55
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.07	0.55
1:B:650:GLN:HE22	1:B:653:LYS:HZ1	1.55	0.55
1:A:1019:ARG:NH1	1:B:1181:LYS:H	2.01	0.55
1:A:1181:LYS:O	1:A:1182:ALA:HB3	2.07	0.55
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.05	0.55
1:A:691:GLN:NE2	1:A:727:LYS:H	2.04	0.55
1:A:27:ILE:HD11	1:A:1013:PHE:CE2	2.41	0.54
1:A:558:ARG:HG2	1:A:560:ASN:HD21	1.72	0.54
1:A:1188:PHE:CE1	1:A:1196:THR:HG23	2.42	0.54
1:B:27:ILE:HD12	1:B:1013:PHE:CE2	2.41	0.54
1:A:976:HIS:HD2	1:B:1003:LYS:HZ2	1.55	0.54
1:A:1175:PHE:CD2	1:B:1151:GLN:HG3	2.43	0.54
1:B:163:SER:O	1:B:164:ASN:HB2	2.07	0.54
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.90	0.54
1:A:841:SER:HA	1:A:844:TRP:CE2	2.43	0.54
1:A:775:VAL:N	1:A:776:PRO:HD2	2.23	0.54
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.38	0.53
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.91	0.53
1:A:692:CYS:O	1:A:693:ASN:HB2	2.08	0.53
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.90	0.53
1:B:495:VAL:HG12	1:B:527:PRO:HD3	1.91	0.53
1:A:565:THR:HG21	1:A:609:ALA:HB3	1.91	0.53
1:A:554:GLY:HA3	1:A:601:MET:HE2	1.91	0.52
1:A:9:ASP:HA	1:A:179:GLU:O	2.09	0.52
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.39	0.52
1:A:1143:GLU:HG2	1:A:1144:ASP:H	1.75	0.52
1:B:841:SER:HA	1:B:844:TRP:CE2	2.44	0.52
7:A:2252:HOH:O	1:B:1219:THR:HG21	2.09	0.52
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.40	0.52
1:B:1219:THR:HG22	1:B:1221:GLU:N	2.25	0.52
1:A:976:HIS:CD2	1:B:1003:LYS:HZ2	2.27	0.52
1:A:536:ASN:HA	1:A:623:LYS:HZ3	1.74	0.52
1:B:581:ASP:O	1:B:585:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:GLU:OE2	1:B:1193:GLU:N	2.43	0.51
1:A:1199:ASP:HB3	7:A:2395:HOH:O	2.10	0.51
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.74	0.51
1:B:964:GLY:O	1:B:968:ASP:HB2	2.10	0.51
1:A:1165:HIS:CD2	1:B:1165:HIS:NE2	2.79	0.51
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.92	0.51
1:B:483:ARG:HA	1:B:503:GLY:O	2.11	0.51
1:B:99:LYS:O	1:B:103:GLU:HG3	2.11	0.51
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.07	0.51
1:A:1200:THR:HG21	1:A:1202:MET:HB2	1.92	0.50
1:B:729:LYS:O	1:B:732:LYS:HG3	2.11	0.50
1:A:1166:MET:O	1:A:1169:THR:HG22	2.12	0.50
1:A:1043:GLY:HA3	1:A:1087:MET:HB2	1.94	0.50
1:B:833:PHE:HE1	1:B:955:LYS:HG3	1.76	0.50
1:A:1007:THR:OG1	1:A:1021:GLY:HA2	2.11	0.50
1:B:978:LEU:O	1:B:1062:PRO:HG2	2.10	0.50
1:A:121:LEU:C	1:A:121:LEU:HD23	2.31	0.50
1:A:561:MET:HE1	1:A:564:GLN:HG2	1.94	0.50
1:A:1105:LEU:O	1:A:1108:GLN:HG2	2.10	0.50
1:A:1219:THR:CG2	1:A:1221:GLU:H	2.22	0.50
1:A:441:ILE:HD13	1:A:573:VAL:HG21	1.93	0.50
1:B:121:LEU:HD23	1:B:121:LEU:C	2.31	0.50
1:B:1210:GLU:HG3	7:B:2546:HOH:O	2.11	0.50
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.93	0.50
1:A:636:ASN:ND2	1:A:672:PHE:CE1	2.80	0.50
1:B:56:LEU:HD23	1:B:58:ILE:CD1	2.42	0.50
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.47	0.50
1:A:12:THR:CG2	1:A:39:GLU:OE1	2.60	0.50
1:A:351:ARG:HD2	7:A:2154:HOH:O	2.12	0.50
1:B:632:GLU:O	1:B:632:GLU:CD	2.50	0.49
1:A:609:ALA:O	1:A:613:LEU:HB2	2.13	0.49
1:A:964:GLY:O	1:A:968:ASP:HB2	2.12	0.49
1:A:1219:THR:CG2	1:A:1220:SER:N	2.74	0.49
1:A:434:ASN:ND2	1:A:466:SER:OG	2.45	0.49
1:A:421:GLN:HA	1:A:466:SER:O	2.13	0.49
1:B:690:ILE:HG12	2:B:1233:SF4:S2	2.52	0.49
1:B:1043:GLY:HA3	1:B:1087:MET:HB2	1.94	0.49
1:A:297:ILE:HB	1:A:379:TYR:CE2	2.47	0.49
1:A:553:VAL:O	1:A:601:MET:HE2	2.13	0.49
1:A:6:MET:CE	1:A:185:VAL:HG11	2.43	0.49
1:A:3:LYS:HG2	1:A:184:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:SER:HA	1:A:129:ASP:HB3	1.94	0.48
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.95	0.48
1:A:635:THR:CG2	1:A:639:PHE:HB3	2.43	0.48
1:A:918:ASN:HA	1:A:954:LYS:HD3	1.94	0.48
1:A:222:PRO:HD3	1:B:124:PHE:CE2	2.49	0.48
1:A:1015:ALA:HB3	1:B:1185:SER:HB2	1.95	0.48
1:A:583:LEU:O	1:A:587:ILE:HG13	2.13	0.48
1:B:467:HIS:CE1	1:B:480:LEU:HD22	2.48	0.48
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.13	0.48
1:A:467:HIS:HB3	1:A:481:VAL:HG23	1.96	0.48
1:B:1026:ALA:O	1:B:1030:MET:HG3	2.13	0.48
1:A:635:THR:HG22	1:A:639:PHE:HB3	1.95	0.48
1:A:483:ARG:O	1:A:505:LYS:HE3	2.13	0.48
1:A:124:PHE:HB3	1:A:367:SER:CB	2.43	0.48
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.48	0.48
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.44	0.48
1:B:495:VAL:HG11	1:B:526:LEU:HD12	1.95	0.48
1:A:422:PHE:HE1	1:A:468:LEU:HG	1.79	0.48
1:A:1214:GLN:O	1:A:1214:GLN:HG2	2.13	0.48
1:A:1136:VAL:HG12	1:A:1139:ARG:NH1	2.28	0.48
1:B:650:GLN:NE2	1:B:653:LYS:HZ3	2.12	0.48
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.14	0.48
3:A:1236:HTL:H4'2	3:A:1236:HTL:C1'	2.27	0.47
1:A:27:ILE:CD1	1:A:1013:PHE:CE2	2.97	0.47
1:B:1173:GLU:HG2	1:B:1174:SER:H	1.78	0.47
1:A:1143:GLU:HG2	1:A:1144:ASP:N	2.29	0.47
1:A:1132:ASN:O	1:A:1136:VAL:HG22	2.14	0.47
1:A:684:TRP:CE2	1:A:738:ILE:HB	2.49	0.47
1:A:1199:ASP:O	1:B:455:TYR:HB3	2.14	0.47
1:B:27:ILE:CD1	1:B:1013:PHE:CE2	2.98	0.47
1:B:635:THR:CG2	1:B:636:ASN:N	2.77	0.47
1:A:10:GLY:O	1:A:14:THR:CG2	2.63	0.47
1:A:561:MET:O	1:A:561:MET:HE3	2.14	0.47
1:B:427:ALA:HA	7:B:2224:HOH:O	2.14	0.47
1:B:1006:PRO:HG2	1:B:1009:ALA:HB2	1.97	0.47
1:B:12:THR:CG2	1:B:39:GLU:OE1	2.53	0.47
1:A:591:TYR:C	1:A:593:LYS:N	2.68	0.47
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.48	0.47
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	1.97	0.47
1:B:1177:PRO:O	1:B:1178:ALA:HB2	2.15	0.47
1:B:660:GLU:HB3	7:B:2309:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:OH	1:A:298:GLY:HA3	2.15	0.47
1:A:992:GLU:O	1:A:993:VAL:CG1	2.62	0.47
1:B:720:ASN:H	1:B:720:ASN:ND2	2.13	0.47
1:B:1231:LYS:HG3	1:B:1232:LYS:N	2.25	0.47
1:A:707:VAL:HB	1:A:737:ARG:HB3	1.97	0.47
1:B:31:THR:HG1	6:B:1240:CO2:C	2.28	0.47
1:B:1200:THR:HG23	1:B:1202:MET:HE2	1.97	0.46
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.45	0.46
1:A:235:TYR:O	1:A:239:VAL:HG12	2.14	0.46
1:A:949:SER:HA	1:A:952:TYR:CZ	2.50	0.46
1:A:90:LEU:HD21	1:A:168:MET:HE2	1.97	0.46
1:A:1171:ILE:HD12	1:B:1161:LYS:HD3	1.96	0.46
1:B:713:GLU:OE1	1:B:785:PRO:HD2	2.15	0.46
1:B:635:THR:HG22	1:B:636:ASN:O	2.15	0.46
1:B:589:LYS:C	1:B:590:ALA:O	2.52	0.46
1:A:586:SER:O	1:A:589:LYS:HB3	2.16	0.46
1:A:597:LYS:O	1:A:601:MET:HG3	2.15	0.46
1:B:1146:LYS:NZ	7:B:2524:HOH:O	2.48	0.46
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.97	0.46
1:A:513:ASN:ND2	1:A:546:ALA:HB3	2.31	0.46
1:A:642:VAL:O	1:A:646:ILE:HG13	2.15	0.46
1:A:1136:VAL:HG23	1:A:1137:LEU:N	2.31	0.46
1:B:712:GLU:O	1:B:715:VAL:HG23	2.15	0.46
1:A:37:GLY:HA3	7:A:2011:HOH:O	2.17	0.45
1:A:591:TYR:O	1:A:593:LYS:N	2.50	0.45
1:B:1181:LYS:HD2	1:B:1182:ALA:N	2.23	0.45
1:B:27:ILE:HB	7:B:2036:HOH:O	2.16	0.45
1:A:1132:ASN:ND2	1:A:1136:VAL:CG1	2.79	0.45
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.97	0.45
1:B:1219:THR:HG22	1:B:1221:GLU:H	1.81	0.45
1:A:129:ASP:OD2	1:A:130:ILE:N	2.49	0.45
1:A:45:ALA:HB1	1:B:1185:SER:HB3	1.99	0.45
1:B:720:ASN:HD22	1:B:720:ASN:N	2.14	0.45
1:B:87:SER:HA	1:B:129:ASP:HB3	1.99	0.45
1:A:335:ALA:HB2	7:A:2145:HOH:O	2.16	0.45
1:A:775:VAL:O	1:A:779:GLU:HG2	2.16	0.45
1:A:1033:GLY:HA3	1:A:1173:GLU:HG3	1.98	0.45
1:B:692:CYS:O	1:B:693:ASN:HB2	2.17	0.45
1:A:731:LEU:HD23	1:A:790:VAL:HG11	1.98	0.45
1:B:720:ASN:HD22	1:B:720:ASN:H	1.64	0.45
1:A:180:ILE:O	1:A:450:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:HG21	1:B:439:LYS:HA	1.99	0.45
1:B:1173:GLU:HG2	1:B:1174:SER:N	2.32	0.45
1:A:124:PHE:CE2	1:B:222:PRO:HD3	2.52	0.45
1:A:113:ALA:HB1	1:A:126:ASP:O	2.17	0.45
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.51	0.45
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.52	0.45
1:B:9:ASP:HA	1:B:179:GLU:O	2.17	0.44
1:A:1226:LEU:O	1:A:1230:THR:HG23	2.17	0.44
1:B:439:LYS:NZ	1:B:439:LYS:HB2	2.32	0.44
1:A:524:LYS:HD2	1:A:525:HIS:CE1	2.52	0.44
1:A:978:LEU:O	1:A:1062:PRO:HG2	2.17	0.44
1:B:221:ASN:HB3	1:B:222:PRO:HD2	1.98	0.44
1:A:1159:ARG:O	1:A:1163:LEU:HG	2.17	0.44
1:B:12:THR:HG22	1:B:39:GLU:CD	2.35	0.44
1:A:594:LYS:O	1:A:595:GLY:O	2.34	0.44
1:B:1231:LYS:O	1:B:1232:LYS:HB2	2.17	0.44
1:A:444:ASN:CB	1:A:582:LEU:HD21	2.47	0.44
1:A:741:ASN:HA	1:A:778:LEU:HG	1.99	0.44
1:A:1106:ALA:C	1:A:1108:GLN:H	2.20	0.44
1:B:562:ILE:HD12	1:B:562:ILE:H	1.82	0.44
1:A:554:GLY:HA3	1:A:601:MET:HE1	1.97	0.44
1:A:857:ARG:HG3	1:A:858:LEU:HD13	2.00	0.44
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.81	0.44
1:B:212:HIS:HD2	7:B:2087:HOH:O	2.00	0.44
1:B:587:ILE:O	1:B:591:TYR:HB2	2.18	0.44
1:A:26:ALA:HB3	1:A:71:VAL:HG23	2.00	0.43
1:B:684:TRP:CE2	1:B:738:ILE:HB	2.53	0.43
1:A:700:PRO:HG2	1:A:814:GLY:HA2	1.99	0.43
1:A:643:VAL:HB	1:A:849:PRO:HB2	2.01	0.43
1:A:892:ASP:OD1	1:A:896:LYS:NZ	2.48	0.43
1:A:713:GLU:OE1	1:A:785:PRO:HD2	2.18	0.43
1:A:598:ILE:O	1:A:598:ILE:HG22	2.18	0.43
1:A:617:LYS:HD3	1:A:617:LYS:HA	1.86	0.43
1:B:1200:THR:HG23	1:B:1202:MET:CE	2.48	0.43
1:A:233:ASN:HB2	1:A:234:PRO:HD3	2.00	0.43
1:B:1232:LYS:HZ2	1:B:1232:LYS:HB3	1.83	0.43
1:A:389:HIS:CE1	1:B:350:GLU:OE1	2.71	0.43
1:B:441:ILE:HD13	1:B:573:VAL:HG11	2.01	0.43
1:B:210:PRO:O	1:B:213:PRO:HD3	2.19	0.43
1:B:630:LYS:HB2	1:B:632:GLU:HG3	2.00	0.43
1:A:6:MET:HE1	1:A:185:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:VAL:CG1	1:B:527:PRO:HD3	2.48	0.43
1:A:121:LEU:HD23	1:A:122:SER:N	2.34	0.43
1:A:116:ILE:HD11	1:A:129:ASP:HB3	2.00	0.43
1:A:41:ASP:HA	1:A:58:ILE:HD12	2.01	0.43
1:A:84:PHE:HA	1:A:110:HIS:O	2.18	0.43
1:A:1082:LYS:O	1:A:1086:VAL:HG23	2.18	0.43
1:A:391:THR:O	1:A:402:SER:HA	2.18	0.43
1:A:841:SER:O	1:A:845:GLY:HA3	2.19	0.42
1:B:697:PHE:CD2	1:B:1046:LYS:HD3	2.54	0.42
1:A:1218:GLY:N	1:B:747:GLY:O	2.52	0.42
1:B:597:LYS:O	1:B:601:MET:HG3	2.19	0.42
1:A:931:LYS:HE2	1:A:949:SER:HB2	2.00	0.42
1:A:365:LEU:HD22	1:B:226:PHE:CE2	2.54	0.42
1:B:755:CYS:HA	1:B:756:PRO:HD3	1.81	0.42
1:B:20:ALA:HB2	1:B:188:TYR:CE2	2.54	0.42
1:B:1051:LYS:HE2	1:B:1100:ARG:NH1	2.34	0.42
1:A:236:TYR:HA	1:A:239:VAL:CG1	2.49	0.42
1:B:630:LYS:CG	1:B:630:LYS:O	2.67	0.42
1:A:1039:THR:OG1	1:A:1098:LEU:HA	2.20	0.42
1:B:532:ARG:NH1	1:B:625:ALA:O	2.51	0.42
1:B:828:PHE:CE2	1:B:1057:GLU:HG3	2.55	0.42
1:A:562:ILE:N	1:A:562:ILE:HD12	2.34	0.42
1:A:646:ILE:HB	1:A:849:PRO:HG3	2.02	0.42
1:B:994:TYR:HB2	1:B:1000:GLN:HE21	1.84	0.42
1:A:779:GLU:O	1:A:783:ARG:HD3	2.20	0.42
1:A:20:ALA:O	1:A:51:ILE:HG23	2.19	0.42
1:B:130:ILE:O	1:B:140:MET:HE3	2.19	0.42
1:A:110:HIS:CE1	1:A:157:HIS:NE2	2.85	0.42
1:A:521:ASP:O	1:A:524:LYS:HB3	2.20	0.42
1:A:389:HIS:HE1	1:B:350:GLU:CD	2.23	0.42
1:B:110:HIS:CE1	1:B:157:HIS:NE2	2.87	0.42
1:B:143:SER:OG	1:B:169:HIS:HE1	2.03	0.42
1:B:1219:THR:HG22	1:B:1220:SER:N	2.35	0.42
1:A:349:VAL:HG21	1:B:345:CYS:SG	2.59	0.42
1:B:129:ASP:OD2	1:B:130:ILE:N	2.53	0.42
1:A:695:CYS:HB2	1:A:704:ILE:CD1	2.50	0.42
1:B:794:ASP:OD1	1:B:1054:LYS:HD3	2.20	0.42
1:A:573:VAL:HG23	1:A:574:LEU:HG	2.02	0.41
1:A:636:ASN:HD21	1:A:672:PHE:HE1	1.67	0.41
1:A:8:THR:HB	1:A:12:THR:OG1	2.20	0.41
1:A:115:ALA:HB2	1:A:126:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:HIS:HE1	1:B:350:GLU:OE2	2.03	0.41
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.41
1:B:544:ILE:HD12	1:B:613:LEU:HG	2.03	0.41
1:B:617:LYS:HD3	1:B:617:LYS:HA	1.79	0.41
1:A:590:ALA:O	1:A:591:TYR:C	2.59	0.41
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.20	0.41
1:A:794:ASP:OD1	1:A:1054:LYS:NZ	2.48	0.41
1:A:889:HIS:O	1:A:893:LEU:HD22	2.21	0.41
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.49	0.41
1:A:544:ILE:O	1:A:544:ILE:HG23	2.21	0.41
1:A:3:LYS:HG2	1:A:184:GLU:CD	2.40	0.41
1:A:11:ASN:HD22	1:A:11:ASN:HA	1.71	0.41
1:A:408:ALA:O	1:A:409:PHE:C	2.59	0.41
1:A:62:GLN:HB3	1:B:976:HIS:CG	2.55	0.41
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.92	0.41
1:B:961:GLY:HA3	1:B:965:TRP:CE3	2.56	0.41
1:B:131:TYR:CE2	1:B:339:PRO:HB2	2.55	0.41
1:A:88:GLN:HB3	7:A:2032:HOH:O	2.21	0.41
1:A:24:VAL:HG13	1:B:881:MET:CE	2.51	0.41
1:B:124:PHE:HB3	1:B:367:SER:CB	2.51	0.41
1:A:371:SER:HB2	1:A:372:PRO:HD2	2.03	0.41
1:A:701:HIS:CE1	1:A:746:MET:HG3	2.56	0.41
1:A:646:ILE:HD12	1:A:849:PRO:HB3	2.03	0.41
1:B:1055:GLU:O	1:B:1104:ARG:NH1	2.54	0.41
1:B:235:TYR:O	1:B:239:VAL:HG23	2.21	0.41
1:A:1000:GLN:H	1:A:1000:GLN:NE2	2.18	0.41
1:B:949:SER:C	1:B:951:LEU:H	2.24	0.41
1:B:857:ARG:NH1	7:B:2393:HOH:O	2.53	0.41
1:B:786:VAL:HG12	1:B:801:PHE:O	2.21	0.41
1:B:869:PHE:CZ	3:B:1236:HTL:H5B2	2.56	0.40
7:A:2205:HOH:O	1:B:1199:ASP:HB3	2.21	0.40
1:B:1221:GLU:HB2	7:B:2552:HOH:O	2.20	0.40
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	2.03	0.40
1:A:712:GLU:O	1:A:715:VAL:HG23	2.21	0.40
1:B:456:ASP:OD2	1:B:457:SER:N	2.54	0.40
1:B:1124:VAL:O	1:B:1128:LEU:HG	2.21	0.40
1:B:115:ALA:HA	1:B:126:ASP:OD2	2.21	0.40
1:B:978:LEU:HD23	1:B:978:LEU:HA	1.88	0.40
1:A:695:CYS:HB2	1:A:704:ILE:HD13	2.03	0.40
1:A:956:SER:HG	1:A:958:TRP:HE1	1.70	0.40
1:A:754:ILE:C	1:A:754:ILE:HD12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:NE	1:B:123:ILE:HA	2.36	0.40
1:B:1200:THR:HG22	1:B:1202:MET:HB2	2.02	0.40
1:A:1200:THR:HA	1:A:1201:PRO:HD3	1.93	0.40
1:A:593:LYS:CG	1:A:594:LYS:N	2.73	0.40
1:B:727:LYS:HG3	1:B:728:GLY:N	2.37	0.40
1:A:1077:ARG:HG2	1:A:1130:ALA:C	2.41	0.40
1:A:523:ASP:HA	1:A:531:LYS:HZ3	1.87	0.40
1:A:709:ALA:HB3	1:A:714:LEU:HD21	2.03	0.40
1:A:1230:THR:O	1:A:1232:LYS:N	2.54	0.40
1:B:695:CYS:HB2	1:B:704:ILE:CD1	2.51	0.40
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.37	0.40
1:A:737:ARG:HE	1:A:739:GLN:HE21	1.66	0.40
1:A:426:GLY:HA3	1:B:1199:ASP:CG	2.42	0.40
1:B:411:ASP:HB2	1:B:483:ARG:HD2	2.03	0.40
1:A:117:ALA:HB1	1:B:99:LYS:HE2	2.04	0.40
1:B:794:ASP:N	1:B:794:ASP:OD2	2.52	0.40
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.96	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	1229/1231 (100%)	1157 (94%)	65 (5%)	7 (1%)	30	41
1	B	1229/1231 (100%)	1175 (96%)	44 (4%)	10 (1%)	24	33
All	All	2458/2462 (100%)	2332 (95%)	109 (4%)	17 (1%)	26	37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1231	LYS

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Mol	Chain	Res	Type
1	B	629	THR
1	B	1181	LYS
1	B	1231	LYS
1	A	595	GLY
1	A	1178	ALA
1	A	1181	LYS
1	B	732	LYS
1	B	591	TYR
1	B	1178	ALA
1	B	1182	ALA
1	B	590	ALA
1	B	1174	SER
1	A	577	GLU
1	A	592	GLY
1	A	715	VAL
1	B	592	GLY

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	978/978 (100%)	944 (96%)	34 (4%)	43	63
1	B	978/978 (100%)	953 (97%)	25 (3%)	54	74
All	All	1956/1956 (100%)	1897 (97%)	59 (3%)	48	69

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	12	THR
1	A	14	THR
1	A	154	LEU
1	A	175	ARG
1	A	194	LEU
1	A	204	ARG

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Mol	Chain	Res	Type
1	A	226	PHE
1	A	239	VAL
1	A	317	LEU
1	A	327	LEU
1	A	349	VAL
1	A	351	ARG
1	A	570	LEU
1	A	582	LEU
1	A	613	LEU
1	A	617	LYS
1	A	624	ASP
1	A	632	GLU
1	A	634	MET
1	A	643	VAL
1	A	730	GLU
1	A	808	PHE
1	A	849	PRO
1	A	858	LEU
1	A	893	LEU
1	A	942	LEU
1	A	953	THR
1	A	1000	GLN
1	A	1077	ARG
1	A	1088	ASN
1	A	1170	ASN
1	A	1183	ASP
1	A	1196	THR
1	B	7	THR
1	B	194	LEU
1	B	226	PHE
1	B	290	LEU
1	B	317	LEU
1	B	342	LEU
1	B	359	LEU
1	B	463	ILE
1	B	509	THR
1	B	514	SER
1	B	583	LEU
1	B	620	ASP
1	B	624	ASP
1	B	632	GLU
1	B	635	THR

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Mol	Chain	Res	Type
1	B	720	ASN
1	B	754	ILE
1	B	823	VAL
1	B	836	ASN
1	B	849	PRO
1	B	939	ASP
1	B	1000	GLN
1	B	1088	ASN
1	B	1181	LYS
1	B	1183	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	110	HIS
1	A	164	ASN
1	A	169	HIS
1	A	212	HIS
1	A	220	GLN
1	A	289	HIS
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	513	ASN
1	A	525	HIS
1	A	536	ASN
1	A	543	ASN
1	A	560	ASN
1	A	602	ASN
1	A	641	ASN
1	A	683	GLN
1	A	691	GLN
1	A	739	GLN
1	A	765	GLN
1	A	777	ASN
1	A	836	ASN
1	A	866	ASN
1	A	976	HIS

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Mol	Chain	Res	Type
1	A	1000	GLN
1	A	1088	ASN
1	A	1165	HIS
1	A	1170	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	110	HIS
1	B	135	GLN
1	B	169	HIS
1	B	212	HIS
1	B	434	ASN
1	B	467	HIS
1	B	588	HIS
1	B	650	GLN
1	B	688	ASN
1	B	691	GLN
1	B	720	ASN
1	B	976	HIS
1	B	1000	GLN
1	B	1047	GLN
1	B	1088	ASN
1	B	1108	GLN
1	B	1151	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](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	SF4	A	1233	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1234	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1235	1	0,12,12	0.00	-	0,24,24	0.00	-
3	HTL	A	1236	4	22,30,30	3.09	12 (54%)	33,45,45	3.55	11 (33%)
6	CO2	A	1240	-	0,2,2	0.00	-	0,1,1	0.00	-
2	SF4	B	1233	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1234	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1235	1	0,12,12	0.00	-	0,24,24	0.00	-
3	HTL	B	1236	4	22,30,30	3.41	13 (59%)	33,45,45	3.53	12 (36%)
6	CO2	B	1240	-	0,2,2	0.00	-	0,1,1	0.00	-

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	SF4	A	1233	1	-	0/0/48/48	0/6/5/5
2	SF4	A	1234	1	-	0/0/48/48	0/6/5/5
2	SF4	A	1235	1	-	0/0/48/48	0/6/5/5
3	HTL	A	1236	4	-	0/16/21/21	0/2/2/2
6	CO2	A	1240	-	-	0/0/0/0	0/0/0/0
2	SF4	B	1233	1	-	0/0/48/48	0/6/5/5
2	SF4	B	1234	1	-	0/0/48/48	0/6/5/5
2	SF4	B	1235	1	-	0/0/48/48	0/6/5/5
3	HTL	B	1236	4	-	0/16/21/21	0/2/2/2
6	CO2	B	1240	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1236	HTL	P2-O23	-5.27	1.35	1.54
3	B	1236	HTL	C4-N3	-4.26	1.30	1.39
3	A	1236	HTL	C2'-N3'	-3.22	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1236	HTL	C2'-N3'	-3.17	1.28	1.34
3	A	1236	HTL	O5G-C5B	-3.05	1.32	1.44
3	B	1236	HTL	C35-C5'	-2.64	1.45	1.51
3	B	1236	HTL	O5G-C5B	-2.49	1.34	1.44
3	A	1236	HTL	P2-O22	-2.11	1.47	1.54
3	B	1236	HTL	C5A-C5B	-2.11	1.44	1.51
3	A	1236	HTL	P1-O12	2.43	1.60	1.51
3	A	1236	HTL	C6'-N1'	3.19	1.41	1.34
3	A	1236	HTL	P2-O21	3.25	1.61	1.51
3	B	1236	HTL	C6'-N1'	3.31	1.41	1.34
3	A	1236	HTL	C5'-C4'	3.63	1.51	1.42
3	A	1236	HTL	O2'-C1'	3.66	1.35	1.22
3	B	1236	HTL	C3'-C1'	3.75	1.61	1.49
3	B	1236	HTL	C4'-N3'	4.53	1.42	1.35
3	B	1236	HTL	C5-S1	4.69	1.82	1.74
3	B	1236	HTL	O2'-C1'	4.76	1.39	1.22
3	A	1236	HTL	C2'-N1'	5.04	1.43	1.34
3	A	1236	HTL	C5-S1	5.43	1.84	1.74
3	A	1236	HTL	C4'-N3'	5.48	1.43	1.35
3	A	1236	HTL	C4A-C4	6.00	1.62	1.49
3	B	1236	HTL	C2'-N1'	6.26	1.45	1.34
3	B	1236	HTL	C4A-C4	6.30	1.63	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1236	HTL	C5A-C5-C4	-12.99	115.92	127.56
3	A	1236	HTL	C5A-C5-C4	-11.41	117.34	127.56
3	A	1236	HTL	C35-N3-C2	-9.34	113.42	126.08
3	A	1236	HTL	C5A-C5-S1	-7.60	109.60	120.24
3	B	1236	HTL	C5A-C5-S1	-7.06	110.35	120.24
3	B	1236	HTL	C35-N3-C2	-6.29	117.55	126.08
3	A	1236	HTL	C5'-C35-N3	-4.91	105.17	113.31
3	B	1236	HTL	N1'-C2'-N3'	-4.03	118.14	125.60
3	A	1236	HTL	N1'-C2'-N3'	-3.70	118.75	125.60
3	B	1236	HTL	N4'-C4'-N3'	-3.12	112.42	116.95
3	B	1236	HTL	C4A-C4-C5	-2.26	123.83	128.90
3	A	1236	HTL	C4A-C4-C5	-2.03	124.34	128.90
3	B	1236	HTL	O5G-C5B-C5A	2.29	118.86	109.30
3	B	1236	HTL	C6'-N1'-C2'	2.87	120.79	115.77
3	A	1236	HTL	C2'-N3'-C4'	2.92	124.00	118.19
3	A	1236	HTL	O5G-C5B-C5A	3.01	121.88	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1236	HTL	C2'-N3'-C4'	3.05	124.25	118.19
3	B	1236	HTL	C5'-C4'-N4'	3.07	126.76	122.25
3	B	1236	HTL	C4A-C4-N3	3.24	127.11	122.82
3	A	1236	HTL	C6'-N1'-C2'	3.37	121.66	115.77
3	A	1236	HTL	O23-P2-O22	3.44	120.50	107.38
3	A	1236	HTL	C2A-C2'-N1'	5.53	123.67	117.03
3	B	1236	HTL	C2A-C2'-N1'	7.87	126.48	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1236	HTL	2	0
2	B	1233	SF4	1	0
3	B	1236	HTL	2	0
6	B	1240	CO2	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	1231/1231 (100%)	0.13	90 (7%) 18 17	6, 23, 63, 111	0
1	B	1231/1231 (100%)	-0.19	31 (2%) 61 60	5, 17, 47, 99	0
All	All	2462/2462 (100%)	-0.03	121 (4%) 33 33	5, 19, 57, 111	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1175	PHE	9.1
1	A	1174	SER	9.0
1	A	1177	PRO	8.9
1	B	1232	LYS	8.5
1	A	1232	LYS	6.7
1	A	629	THR	6.6
1	B	1177	PRO	6.5
1	A	619	PRO	6.3
1	B	631	ALA	6.0
1	A	1176	ALA	5.8
1	A	590	ALA	5.6
1	A	626	PRO	5.4
1	A	591	TYR	5.3
1	A	576	PHE	5.3
1	A	1178	ALA	5.3
1	A	594	LYS	5.3
1	A	630	LYS	5.3
1	A	592	GLY	5.1
1	A	621	SER	5.1
1	A	589	LYS	5.0
1	B	1176	ALA	4.9
1	A	535	ALA	4.9
1	A	627	ALA	4.9
1	B	1175	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	633	PRO	4.7
1	B	1178	ALA	4.7
1	A	625	ALA	4.6
1	A	554	GLY	4.6
1	A	596	GLU	4.6
1	A	598	ILE	4.5
1	A	577	GLU	4.4
1	A	628	GLU	4.4
1	A	593	LYS	4.4
1	A	524	LYS	4.3
1	B	1183	ASP	4.2
1	A	1165	HIS	4.1
1	A	599	VAL	4.1
1	A	520	GLU	4.1
1	A	616	PHE	4.1
1	A	600	LYS	4.0
1	B	1230	THR	3.9
1	A	758	LYS	3.9
1	A	1231	LYS	3.8
1	B	1231	LYS	3.7
1	A	595	GLY	3.7
1	A	620	ASP	3.7
1	A	618	TYR	3.7
1	A	634	MET	3.6
1	B	1165	HIS	3.5
1	A	597	LYS	3.5
1	A	623	LYS	3.4
1	A	622	TRP	3.4
1	A	624	ASP	3.4
1	A	631	ALA	3.3
1	A	588	HIS	3.3
1	A	519	LEU	3.3
1	A	523	ASP	3.3
1	B	1181	LYS	3.3
1	A	517	SER	3.2
1	A	521	ASP	3.2
1	B	292	ALA	3.1
1	B	1228	LYS	3.1
1	B	1179	GLY	3.1
1	A	603	THR	3.0
1	A	1173	GLU	3.0
1	A	608	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	530	ILE	2.9
1	A	553	VAL	2.9
1	A	632	GLU	2.8
1	A	936	GLY	2.8
1	B	1227	SER	2.8
1	A	522	MET	2.8
1	A	1179	GLY	2.8
1	B	1174	SER	2.8
1	A	1172	PHE	2.8
1	A	716	GLY	2.7
1	B	629	THR	2.7
1	B	291	ALA	2.7
1	B	717	ALA	2.7
1	A	580	VAL	2.6
1	A	552	ASP	2.6
1	A	712	GLU	2.6
1	A	1180	GLY	2.6
1	A	551	THR	2.5
1	A	532	ARG	2.5
1	A	756	PRO	2.5
1	A	734	TYR	2.5
1	B	1221	GLU	2.5
1	A	715	VAL	2.5
1	A	587	ILE	2.5
1	A	727	LYS	2.4
1	A	609	ALA	2.4
1	B	1173	GLU	2.4
1	B	1171	ILE	2.4
1	A	717	ALA	2.4
1	A	528	SER	2.4
1	B	596	GLU	2.4
1	A	604	ASP	2.3
1	A	601	MET	2.3
1	A	726	ALA	2.3
1	A	725	GLU	2.3
1	B	593	LYS	2.3
1	A	575	PRO	2.3
1	A	518	SER	2.3
1	A	780	TYR	2.3
1	A	611	THR	2.2
1	A	1169	THR	2.2
1	A	1182	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	685	VAL	2.2
1	A	538	LYS	2.2
1	A	555	LEU	2.2
1	B	92	LEU	2.2
1	A	714	LEU	2.2
1	B	712	GLU	2.2
1	A	1230	THR	2.2
1	A	733	GLY	2.1
1	B	937	GLN	2.1
1	B	688	ASN	2.1
1	B	1180	GLY	2.0
1	B	599	VAL	2.0
1	A	901	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 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
6	CO2	A	1240	3/3	0.91	0.40	5.49	38,38,42,46	0
5	CA	A	1239	1/1	0.96	0.16	3.25	58,58,58,58	0
6	CO2	B	1240	3/3	0.97	0.29	2.34	29,29,31,31	0
3	HTL	A	1236	29/29	0.96	0.19	0.24	10,21,38,40	0
3	HTL	B	1236	29/29	0.97	0.17	-0.10	8,12,25,27	0
5	CA	B	1239	1/1	0.96	0.09	-1.51	58,58,58,58	0
2	SF4	A	1233	8/8	0.97	0.11	-1.62	30,31,32,33	0
2	SF4	A	1234	8/8	0.97	0.07	-2.12	22,25,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SF4	B	1233	8/8	0.97	0.06	-2.16	15,18,20,20	0
4	MG	A	1238	1/1	0.98	0.07	-2.29	9,9,9,9	0
2	SF4	B	1234	8/8	0.98	0.06	-2.63	14,15,16,17	0
4	MG	B	1238	1/1	0.99	0.06	-3.20	3,3,3,3	0
2	SF4	A	1235	8/8	0.97	0.05	-3.30	17,19,22,22	0
2	SF4	B	1235	8/8	0.98	0.05	-3.48	7,10,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.