



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:16 PM GMT

PDB ID : 1WYG
Title : Crystal Structure of a Rat Xanthine Dehydrogenase Triple Mutant (C535A, C992R and C1324S)
Authors : Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Hori, H.; Matsumura, T.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2005-02-14
Resolution : 2.60 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

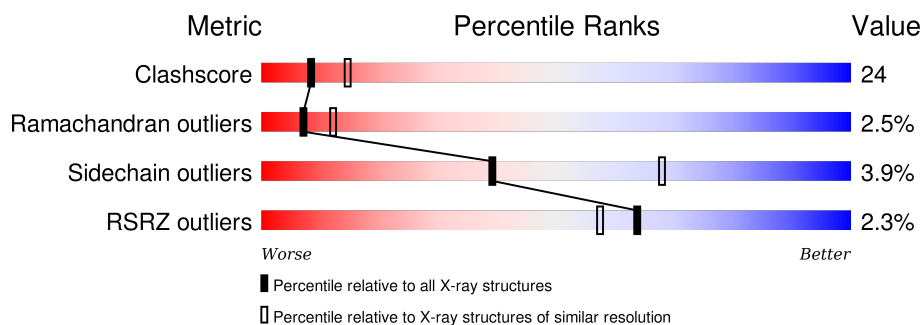
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	1331	

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
4	FES	A	4002	-	-	X	-
6	SAL	A	4005	-	-	-	X
7	ACY	A	3001	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10330 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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1297	Total	C	N	O	S	0	0	0
			10033	6359	1730	1882	62			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P22985
A	535	ALA	CYS	ENGINEERED	UNP P22985
A	992	ARG	CYS	ENGINEERED	UNP P22985
A	1324	SER	CYS	ENGINEERED	UNP P22985

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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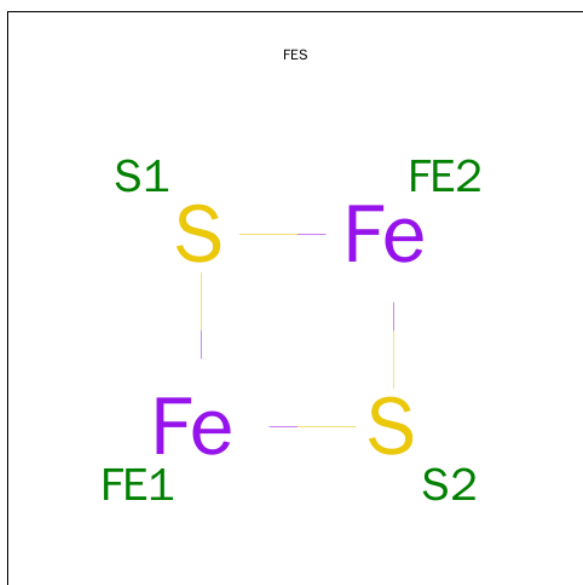
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



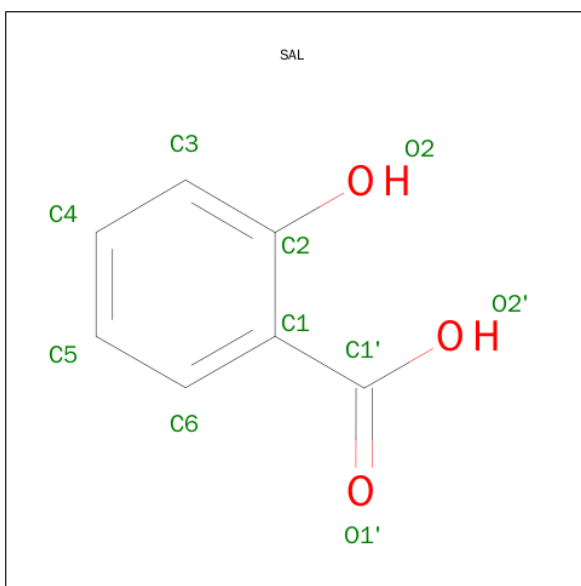
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

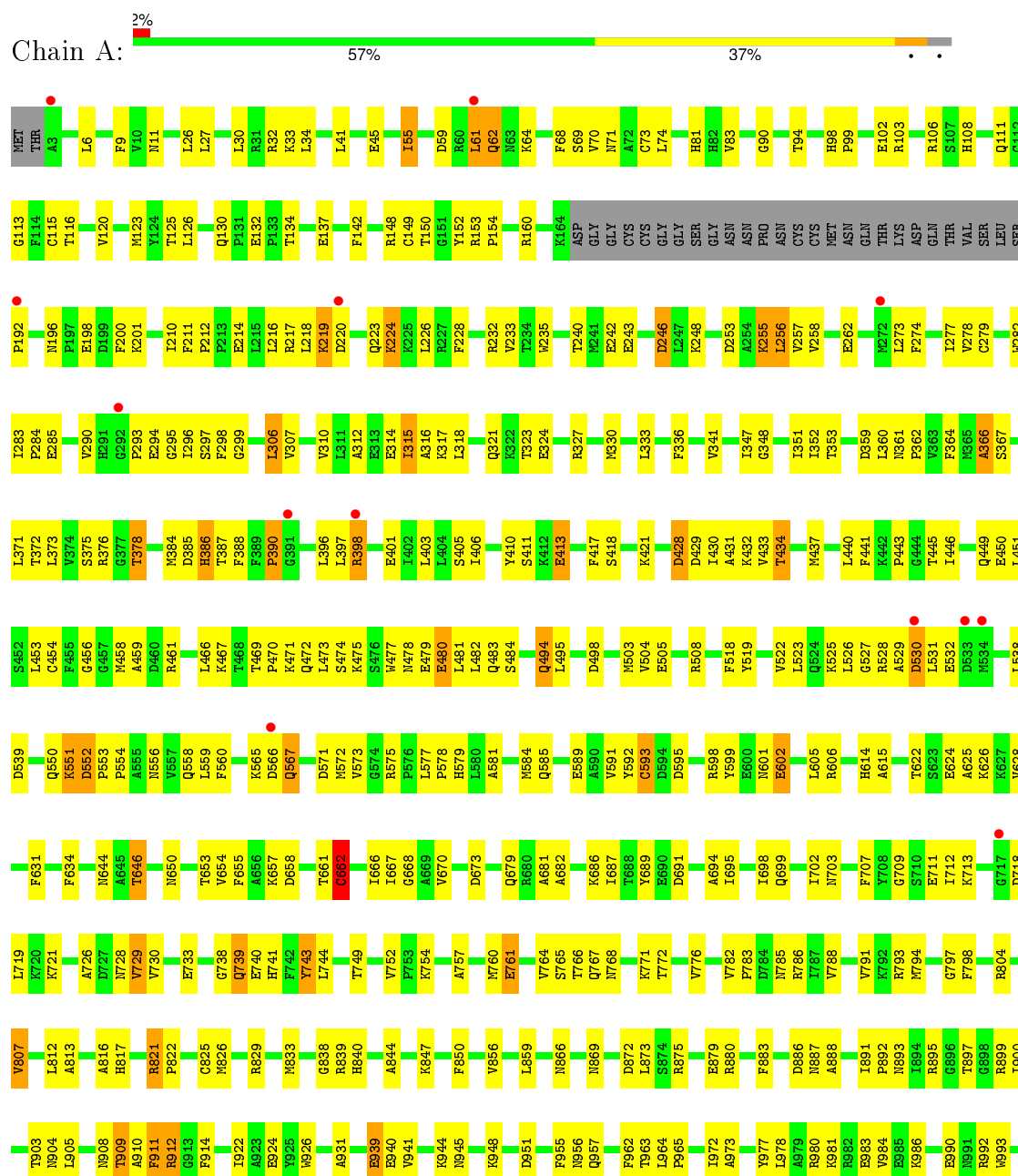
- Molecule 8 is water.

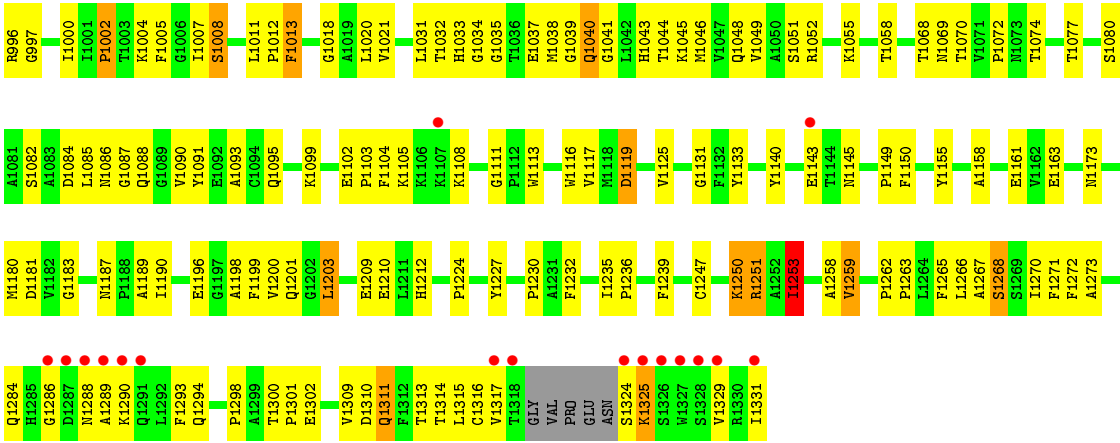
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total	O	0	0
			206	206		

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: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.25Å 134.25Å 523.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 19.91 – 2.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.60) 91.9 (19.91-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.248 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 71082 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAL, PO4, FES, ACY, CA, FAD

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	0.38	0/10244	0.64	0/13859

There are no bond length outliers.

There are no bond angle outliers.

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	10033	0	10046	485	0
2	A	15	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	0	3	0
5	A	53	0	31	3	0
6	A	10	0	5	0	0
7	A	4	0	3	0	0
8	A	206	0	0	5	0
All	All	10330	0	10085	486	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 24.

All (486) 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:766:THR:HG22	1:A:768:ASN:H	0.99	1.08
1:A:1038:MET:H	1:A:1040:GLN:NE2	1.56	1.02
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.27	0.99
1:A:196:ASN:OD1	1:A:198:GLU:HB3	1.63	0.97
1:A:602:GLU:HG2	1:A:822:PRO:HB2	1.45	0.97
1:A:494:GLN:HA	1:A:508:ARG:HH12	1.32	0.95
1:A:766:THR:HG22	1:A:768:ASN:N	1.82	0.94
1:A:1004:LYS:HG3	1:A:1155:TYR:HE2	1.32	0.92
1:A:1311:GLN:HE21	1:A:1311:GLN:H	0.97	0.91
1:A:371:LEU:HD22	1:A:406:ILE:HD12	1.51	0.91
1:A:298:PHE:HE2	1:A:310:VAL:HG11	1.36	0.91
1:A:1033:HIS:HB2	1:A:1086:ASN:HD22	1.34	0.90
1:A:432:LYS:HE3	1:A:503:MET:SD	2.12	0.89
1:A:398:ARG:HB3	1:A:398:ARG:NH1	1.88	0.89
1:A:711:GLU:HB3	1:A:899:ARG:HH11	1.35	0.88
1:A:403:LEU:HD21	1:A:406:ILE:HD11	1.56	0.88
1:A:1173:ASN:ND2	1:A:1270:ILE:HD13	1.91	0.85
1:A:494:GLN:HA	1:A:508:ARG:NH1	1.92	0.84
1:A:718:ASP:H	1:A:893:ASN:ND2	1.77	0.83
1:A:55:ILE:C	1:A:55:ILE:HD13	2.00	0.82
1:A:749:THR:HB	1:A:812:LEU:HD12	1.62	0.81
1:A:963:THR:HG22	1:A:1155:TYR:HD1	1.43	0.80
1:A:821:ARG:HH11	1:A:821:ARG:HB3	1.46	0.79
1:A:1038:MET:H	1:A:1040:GLN:HE22	1.30	0.79
1:A:605:LEU:HD13	1:A:812:LEU:HD23	1.65	0.78
1:A:1311:GLN:NE2	1:A:1311:GLN:H	1.78	0.77
1:A:614:HIS:HB2	1:A:904:ASN:ND2	2.01	0.77
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.66	0.76
1:A:32:ARG:HD2	1:A:598:ARG:CZ	2.15	0.76
1:A:718:ASP:HB3	1:A:721:LYS:HE2	1.67	0.76
1:A:11:ASN:OD1	1:A:90:GLY:HA3	1.84	0.76
1:A:45:GLU:OE1	1:A:1224:PRO:HD2	1.87	0.75
1:A:375:SER:HB3	1:A:378:THR:OG1	1.86	0.75
1:A:55:ILE:HD12	1:A:68:PHE:CZ	2.22	0.75
1:A:821:ARG:HH11	1:A:821:ARG:CB	2.00	0.75
1:A:1311:GLN:N	1:A:1311:GLN:HE21	1.80	0.74
1:A:103:ARG:HG2	1:A:200:PHE:CD1	2.23	0.73
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.53	0.73
1:A:1032:THR:HG21	1:A:1070:THR:HB	1.69	0.73
1:A:963:THR:HG22	1:A:1155:TYR:CD1	2.23	0.73
1:A:1108:LYS:HG2	1:A:1111:GLY:HA3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASP:OD1	1:A:387:THR:HG22	1.89	0.72
1:A:388:PHE:HA	1:A:396:LEU:HG	1.70	0.72
1:A:192:PRO:HB2	1:A:560:PHE:CZ	2.25	0.72
1:A:646:THR:O	1:A:650:ASN:HA	1.90	0.71
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.26	0.71
1:A:216:LEU:O	1:A:219:LYS:HG3	1.91	0.71
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.37	0.70
1:A:298:PHE:CE2	1:A:310:VAL:HG11	2.25	0.70
1:A:306:LEU:O	1:A:310:VAL:HG12	1.91	0.70
1:A:872:ASP:OD1	1:A:909:THR:HG22	1.91	0.70
1:A:718:ASP:H	1:A:893:ASN:HD22	1.38	0.70
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.12	0.70
1:A:766:THR:HG22	1:A:767:GLN:N	2.06	0.69
1:A:957:GLN:OE1	1:A:1149:PRO:HD2	1.93	0.69
1:A:1250:LYS:HD3	1:A:1251:ARG:H	1.57	0.69
1:A:467:LYS:O	1:A:470:PRO:HD2	1.93	0.69
1:A:875:ARG:O	1:A:879:GLU:HG3	1.92	0.69
1:A:565:LYS:HD3	1:A:565:LYS:H	1.57	0.69
1:A:622:THR:HG22	1:A:626:LYS:HG3	1.75	0.69
1:A:290:VAL:HG23	1:A:297:SER:HB2	1.75	0.69
1:A:102:GLU:OE1	1:A:201:LYS:HG2	1.93	0.69
1:A:1113:TRP:O	1:A:1117:VAL:HG23	1.92	0.69
1:A:622:THR:HG23	1:A:625:ALA:HB3	1.75	0.68
1:A:347:ILE:HG13	1:A:348:GLY:H	1.58	0.68
1:A:324:GLU:HB2	1:A:411:SER:CB	2.24	0.68
1:A:1289:ALA:O	1:A:1290:LYS:HB3	1.92	0.68
1:A:662:CYS:HB3	1:A:869:ASN:ND2	2.09	0.68
1:A:498:ASP:HB2	1:A:1325:LYS:HG3	1.75	0.68
1:A:1004:LYS:HG3	1:A:1155:TYR:CE2	2.23	0.67
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.77	0.67
1:A:1173:ASN:HD22	1:A:1270:ILE:HD13	1.58	0.67
1:A:606:ARG:HD3	1:A:679:GLN:HA	1.77	0.67
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.75	0.67
1:A:1044:THR:O	1:A:1048:GLN:HG3	1.95	0.67
1:A:372:THR:O	1:A:373:LEU:HD23	1.95	0.67
1:A:572:MET:HA	1:A:575:ARG:HD2	1.78	0.66
1:A:317:LYS:HG3	1:A:318:LEU:HD12	1.77	0.66
1:A:766:THR:CG2	1:A:768:ASN:H	1.92	0.66
1:A:599:TYR:H	1:A:602:GLU:HG3	1.60	0.66
1:A:1099:LYS:O	1:A:1102:GLU:HG2	1.96	0.66
1:A:451:LEU:HD23	1:A:469:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HG12	1:A:315:ILE:O	1.96	0.65
1:A:530:ASP:C	1:A:532:GLU:H	1.99	0.65
1:A:421:LYS:HE3	1:A:431:ALA:HB2	1.79	0.65
1:A:115:CYS:HB3	1:A:744:LEU:CD1	2.27	0.65
1:A:1035:GLY:H	1:A:1086:ASN:ND2	1.94	0.64
1:A:26:LEU:O	1:A:30:LEU:HG	1.96	0.64
1:A:160:ARG:HH22	1:A:556:ASN:HD21	1.45	0.64
1:A:1203:LEU:C	1:A:1203:LEU:HD12	2.18	0.64
1:A:55:ILE:HG12	1:A:83:VAL:CG1	2.28	0.64
1:A:192:PRO:HB2	1:A:560:PHE:CE1	2.32	0.64
1:A:504:VAL:O	1:A:508:ARG:HG3	1.97	0.64
1:A:405:SER:O	1:A:406:ILE:HD13	1.96	0.64
1:A:872:ASP:OD1	1:A:873:LEU:N	2.31	0.64
1:A:472:GLN:HE21	1:A:481:LEU:HG	1.63	0.64
1:A:880:ARG:NH2	1:A:1150:PHE:HE2	1.96	0.63
1:A:214:GLU:O	1:A:218:LEU:HG	1.97	0.63
1:A:1158:ALA:HB2	1:A:1266:LEU:HB3	1.79	0.63
1:A:398:ARG:CB	1:A:398:ARG:HH11	2.08	0.63
1:A:62:GLN:OE1	1:A:64:LYS:HE2	1.99	0.63
1:A:749:THR:CB	1:A:812:LEU:HD12	2.28	0.63
1:A:360:LEU:HB3	1:A:364:PHE:CE2	2.34	0.62
1:A:1313:THR:O	1:A:1317:VAL:HG13	2.00	0.62
1:A:615:ALA:HB1	1:A:689:TYR:HB3	1.81	0.62
1:A:277:ILE:HG22	1:A:278:VAL:N	2.15	0.62
1:A:1259:VAL:O	1:A:1259:VAL:HG22	1.99	0.62
1:A:142:PHE:HB3	1:A:1232:PHE:CE1	2.35	0.62
4:A:4003:FES:FE1	4:A:4003:FES:S2	1.91	0.62
1:A:565:LYS:HD3	1:A:565:LYS:N	2.15	0.61
1:A:115:CYS:HB3	1:A:744:LEU:HD12	1.81	0.61
1:A:718:ASP:N	1:A:893:ASN:HD22	1.99	0.61
1:A:367:SER:HB3	1:A:417:PHE:HE1	1.65	0.61
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.30	0.61
1:A:295:GLY:HA2	1:A:410:TYR:CE1	2.36	0.61
1:A:324:GLU:HB2	1:A:411:SER:HB3	1.82	0.61
1:A:606:ARG:CD	1:A:679:GLN:HA	2.31	0.61
1:A:224:LYS:H	1:A:224:LYS:HD2	1.65	0.60
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.00	0.60
1:A:584:MET:HG3	8:A:4039:HOH:O	2.01	0.60
1:A:347:ILE:HG13	1:A:348:GLY:N	2.16	0.60
1:A:458:MET:HE3	1:A:495:LEU:HD21	1.83	0.60
1:A:754:LYS:HE2	1:A:761:GLU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NE	1:A:1196:GLU:OE1	2.29	0.60
1:A:741:HIS:HA	1:A:911:PHE:CZ	2.37	0.59
1:A:956:ASN:ND2	1:A:1145:ASN:ND2	2.50	0.59
1:A:518:PHE:O	1:A:522:VAL:HG23	2.03	0.59
1:A:1105:LYS:HG3	1:A:1116:TRP:CZ2	2.37	0.59
1:A:764:VAL:O	1:A:791:VAL:HG22	2.02	0.59
1:A:718:ASP:O	1:A:893:ASN:ND2	2.36	0.59
1:A:98:HIS:ND1	1:A:99:PRO:HD2	2.17	0.59
1:A:955:PHE:HA	1:A:1145:ASN:OD1	2.03	0.59
1:A:712:ILE:HD13	1:A:879:GLU:HG2	1.84	0.58
1:A:232:ARG:NH1	1:A:273:LEU:HD13	2.18	0.58
1:A:359:ASP:CG	1:A:434:THR:HG21	2.23	0.58
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.84	0.58
1:A:255:LYS:HG3	1:A:274:PHE:CD2	2.38	0.58
1:A:992:ARG:NH1	1:A:1284:GLN:HB2	2.18	0.58
1:A:844:ALA:HB2	1:A:922:ILE:CD1	2.33	0.58
1:A:666:ILE:HD12	1:A:807:VAL:HG22	1.85	0.58
1:A:479:GLU:O	1:A:483:GLN:HG2	2.03	0.58
1:A:573:VAL:HG21	1:A:1052:ARG:HD3	1.86	0.58
1:A:508:ARG:NH1	1:A:508:ARG:HG2	2.18	0.58
1:A:323:THR:OG1	1:A:327:ARG:NH1	2.37	0.58
1:A:366:ALA:HB2	1:A:454:CYS:SG	2.44	0.57
1:A:601:ASN:O	1:A:821:ARG:NH1	2.24	0.57
1:A:32:ARG:HD2	1:A:598:ARG:NH1	2.19	0.57
1:A:655:PHE:CD2	1:A:668:GLY:HA2	2.38	0.57
1:A:785:ASN:HB3	1:A:786:ARG:HH11	1.69	0.57
1:A:1038:MET:H	1:A:1040:GLN:HE21	1.48	0.56
1:A:911:PHE:O	1:A:912:ARG:C	2.43	0.56
1:A:739:GLN:HG3	1:A:1209:GLU:OE2	2.04	0.56
1:A:388:PHE:O	1:A:390:PRO:HD3	2.04	0.56
1:A:571:ASP:OD1	1:A:1052:ARG:HD2	2.06	0.56
1:A:566:ASP:O	1:A:567:GLN:C	2.43	0.56
1:A:694:ALA:C	1:A:695:ILE:HD13	2.25	0.56
1:A:718:ASP:CB	1:A:721:LYS:HE2	2.36	0.56
1:A:299:GLY:O	1:A:347:ILE:HD11	2.06	0.56
1:A:529:ALA:O	1:A:530:ASP:HB2	2.06	0.56
1:A:153:ARG:HH11	1:A:153:ARG:HG2	1.71	0.56
1:A:986:LYS:O	1:A:990:GLU:HG3	2.06	0.55
1:A:1209:GLU:HB3	1:A:1227:TYR:CZ	2.40	0.55
1:A:1140:TYR:HB2	1:A:1149:PRO:HB3	1.89	0.55
1:A:760:MET:HE1	1:A:816:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:HG23	1:A:589:GLU:OE2	2.05	0.55
1:A:470:PRO:C	1:A:472:GLN:H	2.10	0.55
1:A:295:GLY:HA2	1:A:410:TYR:CD1	2.41	0.55
1:A:709:GLY:HA3	1:A:875:ARG:NH2	2.22	0.55
1:A:602:GLU:HA	1:A:822:PRO:O	2.07	0.54
1:A:397:LEU:HD12	1:A:397:LEU:H	1.72	0.54
1:A:622:THR:O	1:A:622:THR:HG22	2.07	0.54
1:A:760:MET:HE1	1:A:813:ALA:O	2.08	0.54
1:A:866:ASN:ND2	1:A:1331:ILE:HG23	2.21	0.54
1:A:880:ARG:HH22	1:A:1150:PHE:HE2	1.55	0.54
1:A:472:GLN:HE22	1:A:484:SER:CB	2.21	0.54
1:A:821:ARG:CG	1:A:821:ARG:HH11	2.20	0.54
1:A:525:LYS:HA	1:A:528:ARG:NH1	2.22	0.54
1:A:601:ASN:ND2	1:A:822:PRO:HD3	2.22	0.54
1:A:367:SER:HB3	1:A:417:PHE:CE1	2.42	0.54
1:A:153:ARG:HE	1:A:1196:GLU:CD	2.10	0.54
1:A:565:LYS:CD	1:A:565:LYS:H	2.20	0.54
1:A:1293:PHE:HD2	1:A:1293:PHE:H	1.54	0.54
1:A:371:LEU:CD2	1:A:406:ILE:HG23	2.37	0.54
1:A:504:VAL:HG23	1:A:505:GLU:H	1.74	0.53
1:A:385:ASP:CG	1:A:387:THR:HG22	2.28	0.53
1:A:1105:LYS:HA	1:A:1116:TRP:NE1	2.23	0.53
1:A:103:ARG:HG2	1:A:200:PHE:CE1	2.43	0.53
1:A:879:GLU:O	1:A:883:PHE:CD2	2.62	0.53
1:A:1035:GLY:H	1:A:1086:ASN:HD21	1.54	0.53
1:A:160:ARG:HH22	1:A:556:ASN:ND2	2.05	0.53
1:A:478:ASN:HD21	1:A:480:GLU:HB3	1.73	0.53
1:A:838:GLY:O	1:A:908:ASN:HB3	2.08	0.53
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.91	0.52
1:A:670:VAL:HG21	1:A:682:ALA:HA	1.91	0.52
1:A:599:TYR:C	1:A:601:ASN:N	2.63	0.52
1:A:446:ILE:O	1:A:446:ILE:HG13	2.09	0.52
1:A:1108:LYS:HG2	1:A:1111:GLY:CA	2.38	0.52
1:A:766:THR:CG2	1:A:767:GLN:N	2.72	0.52
1:A:1013:PHE:C	1:A:1013:PHE:CD1	2.83	0.52
1:A:130:GLN:HE21	1:A:132:GLU:H	1.58	0.52
1:A:924:GLU:HB3	1:A:1272:PHE:CE2	2.45	0.52
1:A:1035:GLY:N	1:A:1086:ASN:HD21	2.08	0.52
1:A:698:ILE:HG13	1:A:1331:ILE:OXT	2.10	0.52
1:A:698:ILE:O	1:A:702:ILE:HG13	2.10	0.52
1:A:711:GLU:N	1:A:899:ARG:NH1	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HG3	1:A:434:THR:HG23	1.91	0.51
1:A:33:LYS:O	1:A:33:LYS:HG3	2.10	0.51
1:A:859:LEU:HD22	1:A:926:TRP:CZ2	2.46	0.51
1:A:718:ASP:C	1:A:893:ASN:HD22	2.14	0.51
1:A:964:LEU:HB3	1:A:965:PRO:HD3	1.93	0.51
1:A:469:THR:OG1	1:A:470:PRO:HD3	2.10	0.51
1:A:482:LEU:C	1:A:482:LEU:HD23	2.31	0.51
1:A:856:VAL:HG12	1:A:945:ASN:OD1	2.10	0.51
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.92	0.51
1:A:1265:PHE:O	1:A:1268:SER:HB2	2.10	0.51
1:A:752:VAL:HG13	1:A:752:VAL:O	2.10	0.51
1:A:375:SER:HB2	1:A:401:GLU:HG2	1.91	0.51
1:A:429:ASP:OD1	1:A:430:ILE:N	2.42	0.51
1:A:1158:ALA:CB	1:A:1266:LEU:HB3	2.41	0.50
1:A:277:ILE:HG22	1:A:278:VAL:H	1.76	0.50
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.09	0.50
1:A:223:GLN:NE2	1:A:282:TRP:HB3	2.26	0.50
1:A:599:TYR:HB2	1:A:602:GLU:HG3	1.94	0.50
1:A:503:MET:HG2	1:A:1302:GLU:OE2	2.11	0.50
1:A:606:ARG:NE	1:A:679:GLN:HG3	2.25	0.50
1:A:1045:LYS:HE3	1:A:1190:ILE:HG21	1.94	0.50
1:A:240:THR:OG1	1:A:243:GLU:HG3	2.10	0.50
1:A:527:GLY:HA2	1:A:532:GLU:HA	1.93	0.50
1:A:262:GLU:HB3	5:A:4004:FAD:O2A	2.11	0.50
1:A:673:ASP:OD1	1:A:673:ASP:N	2.42	0.50
1:A:972:ILE:HG13	1:A:973:ALA:N	2.27	0.50
1:A:615:ALA:HA	1:A:691:ASP:HA	1.93	0.50
1:A:428:ASP:OD1	5:A:4004:FAD:H6	2.12	0.50
1:A:760:MET:CE	1:A:816:ALA:HB3	2.42	0.50
1:A:1021:VAL:HG23	1:A:1093:ALA:HB1	1.93	0.50
1:A:498:ASP:HB2	1:A:1325:LYS:O	2.12	0.50
1:A:1140:TYR:CB	1:A:1149:PRO:HB3	2.42	0.50
1:A:98:HIS:CE1	1:A:99:PRO:HD2	2.47	0.50
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.12	0.50
1:A:1262:PRO:HB2	1:A:1263:PRO:HD3	1.92	0.50
1:A:661:THR:O	1:A:662:CYS:HB3	2.12	0.50
1:A:667:ILE:HD13	1:A:687:ILE:HD13	1.92	0.50
1:A:741:HIS:CE1	1:A:838:GLY:HA2	2.47	0.50
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.60	0.49
1:A:1200:VAL:O	1:A:1230:PRO:HG2	2.12	0.49
1:A:601:ASN:HD22	1:A:822:PRO:HD3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:H	1:A:285:GLU:CD	2.15	0.49
1:A:1032:THR:HG21	1:A:1070:THR:CB	2.42	0.49
1:A:478:ASN:ND2	1:A:480:GLU:H	2.10	0.49
1:A:766:THR:HG22	1:A:767:GLN:H	1.74	0.49
1:A:55:ILE:HG12	1:A:83:VAL:HG13	1.93	0.49
1:A:657:LYS:O	1:A:658:ASP:HB2	2.13	0.49
1:A:218:LEU:C	1:A:220:ASP:H	2.15	0.49
1:A:558:GLN:O	1:A:559:LEU:HD23	2.12	0.49
1:A:525:LYS:HA	1:A:528:ARG:HH12	1.76	0.49
1:A:1034:GLY:CA	1:A:1074:THR:HG21	2.42	0.49
1:A:1034:GLY:HA3	1:A:1074:THR:HG21	1.95	0.49
1:A:772:THR:O	1:A:776:VAL:HG23	2.12	0.49
1:A:887:ASN:OD1	1:A:888:ALA:N	2.45	0.49
1:A:812:LEU:HD21	1:A:825:CYS:CB	2.40	0.49
1:A:872:ASP:CG	1:A:909:THR:HG22	2.32	0.49
1:A:472:GLN:NE2	1:A:481:LEU:HG	2.27	0.49
1:A:606:ARG:CZ	1:A:679:GLN:HG3	2.43	0.49
1:A:475:LYS:HD3	1:A:480:GLU:OE2	2.13	0.48
1:A:437:MET:HG2	1:A:453:LEU:HD22	1.94	0.48
1:A:577:LEU:HD12	1:A:578:PRO:HD2	1.94	0.48
1:A:628:VAL:HG21	1:A:681:ALA:HA	1.94	0.48
1:A:59:ASP:OD1	1:A:61:LEU:HB3	2.13	0.48
1:A:255:LYS:HE3	5:A:4004:FAD:O3B	2.14	0.48
1:A:579:HIS:CE1	1:A:581:ALA:HB3	2.48	0.48
1:A:55:ILE:O	1:A:55:ILE:HD13	2.12	0.48
1:A:749:THR:CG2	1:A:812:LEU:HD12	2.44	0.48
1:A:530:ASP:C	1:A:532:GLU:N	2.67	0.48
1:A:634:PHE:CZ	1:A:668:GLY:HA3	2.48	0.48
1:A:210:ILE:HG12	1:A:211:PHE:N	2.29	0.47
1:A:341:VAL:HG23	8:A:4023:HOH:O	2.14	0.47
1:A:1037:GLU:HA	1:A:1040:GLN:HE22	1.78	0.47
1:A:1033:HIS:CE1	1:A:1043:HIS:ND1	2.82	0.47
1:A:1324:SER:O	1:A:1325:LYS:HB2	2.14	0.47
1:A:323:THR:O	1:A:327:ARG:HG3	2.14	0.47
1:A:817:HIS:CG	1:A:817:HIS:O	2.67	0.47
1:A:386:HIS:CG	1:A:466:LEU:HD11	2.50	0.47
1:A:148:ARG:O	1:A:148:ARG:HG3	2.15	0.47
1:A:599:TYR:C	1:A:601:ASN:H	2.18	0.47
1:A:6:LEU:HB2	1:A:228:PHE:CE2	2.49	0.47
1:A:804:ARG:HG2	8:A:4106:HOH:O	2.13	0.47
1:A:579:HIS:HD2	1:A:1041:GLY:HA2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.15	0.47
1:A:1038:MET:N	1:A:1040:GLN:HE22	2.07	0.47
1:A:1046:MET:CE	1:A:1046:MET:HA	2.45	0.47
1:A:909:THR:HB	1:A:910:ALA:H	1.36	0.47
1:A:1046:MET:HE2	1:A:1049:VAL:HG21	1.96	0.47
1:A:553:PRO:HA	1:A:554:PRO:HD3	1.73	0.47
1:A:1005:PHE:HB3	1:A:1262:PRO:HG3	1.96	0.46
1:A:405:SER:C	1:A:406:ILE:HD13	2.36	0.46
1:A:1102:GLU:HG3	1:A:1103:PRO:HD3	1.97	0.46
1:A:744:LEU:HD12	4:A:4002:FES:S2	2.55	0.46
1:A:992:ARG:HG3	1:A:993:TRP:CE2	2.49	0.46
1:A:579:HIS:CD2	1:A:1041:GLY:HA2	2.51	0.46
1:A:70:VAL:HG22	1:A:71:ASN:N	2.30	0.46
1:A:235:TRP:CD1	1:A:235:TRP:C	2.88	0.46
1:A:440:LEU:HB3	1:A:450:GLU:HB2	1.98	0.46
1:A:749:THR:O	1:A:812:LEU:HD13	2.15	0.46
1:A:481:LEU:HD23	1:A:481:LEU:O	2.15	0.46
1:A:667:ILE:CD1	1:A:687:ILE:HD13	2.45	0.46
1:A:45:GLU:OE1	1:A:1224:PRO:CD	2.60	0.46
1:A:440:LEU:HD23	1:A:450:GLU:OE1	2.16	0.46
1:A:551:LYS:O	1:A:552:ASP:CB	2.64	0.46
1:A:866:ASN:HD22	1:A:1331:ILE:HG23	1.80	0.46
1:A:441:PHE:CE1	1:A:526:LEU:HD21	2.51	0.46
1:A:153:ARG:N	1:A:154:PRO:HD2	2.30	0.46
1:A:108:HIS:CE1	1:A:1189:ALA:HB1	2.51	0.46
1:A:1253:ILE:CG2	1:A:1253:ILE:O	2.64	0.46
1:A:315:ILE:HA	1:A:323:THR:HG21	1.98	0.46
1:A:148:ARG:NE	1:A:1201:GLN:HE21	2.14	0.46
1:A:768:ASN:HD21	1:A:771:LYS:CG	2.29	0.46
1:A:149:CYS:HB2	4:A:4002:FES:S1	2.55	0.46
1:A:1309:VAL:HA	1:A:1313:THR:HG21	1.96	0.46
1:A:567:GLN:HE21	1:A:567:GLN:HB3	1.57	0.46
1:A:390:PRO:O	1:A:461:ARG:NH1	2.49	0.45
1:A:55:ILE:CD1	1:A:55:ILE:C	2.74	0.45
1:A:605:LEU:C	1:A:605:LEU:HD23	2.37	0.45
1:A:713:LYS:HG3	1:A:897:THR:HG22	1.98	0.45
1:A:1149:PRO:HG2	1:A:1150:PHE:CD1	2.51	0.45
1:A:470:PRO:O	1:A:473:LEU:HG	2.16	0.45
1:A:709:GLY:HA3	1:A:875:ARG:HH21	1.82	0.45
1:A:503:MET:HE2	1:A:1302:GLU:CD	2.36	0.45
1:A:481:LEU:HD23	1:A:481:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:HA3	1:A:585:GLN:HG2	1.97	0.45
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.80	0.45
1:A:948:LYS:HB2	1:A:951:ASP:OD2	2.16	0.45
1:A:996:ARG:HG2	1:A:1163:GLU:HB2	1.98	0.45
1:A:1259:VAL:O	1:A:1259:VAL:CG2	2.63	0.45
1:A:654:VAL:HG12	1:A:655:PHE:CD1	2.52	0.45
1:A:1031:LEU:HD11	1:A:1090:VAL:HG22	1.99	0.45
1:A:1180:MET:HE1	1:A:1263:PRO:HA	1.99	0.45
1:A:592:TYR:O	1:A:595:ASP:N	2.32	0.45
1:A:1038:MET:HG2	1:A:1040:GLN:NE2	2.32	0.45
1:A:297:SER:HA	1:A:406:ILE:O	2.16	0.45
1:A:738:GLY:O	1:A:739:GLN:HB2	2.16	0.45
1:A:1055:LYS:HE2	1:A:1055:LYS:HB3	1.81	0.45
1:A:757:ALA:O	1:A:786:ARG:HD2	2.17	0.45
1:A:440:LEU:O	1:A:449:GLN:HB3	2.16	0.45
1:A:592:TYR:O	1:A:593:CYS:C	2.56	0.45
1:A:1080:SER:HB3	1:A:1258:ALA:HB1	1.99	0.45
1:A:1051:SER:CB	1:A:1058:THR:HG22	2.46	0.45
1:A:550:GLN:OE1	1:A:550:GLN:HA	2.17	0.44
1:A:153:ARG:HD2	1:A:558:GLN:NE2	2.32	0.44
1:A:33:LYS:O	1:A:34:LEU:HD23	2.17	0.44
1:A:1199:PHE:CE1	1:A:1267:ALA:HA	2.52	0.44
1:A:153:ARG:NH1	1:A:153:ARG:HG2	2.32	0.44
1:A:686:LYS:HB3	1:A:686:LYS:HE3	1.82	0.44
1:A:794:MET:HB2	1:A:794:MET:HE2	1.70	0.44
1:A:905:LEU:HD11	1:A:1331:ILE:HG13	1.99	0.44
1:A:1021:VAL:HG22	1:A:1031:LEU:HD13	1.99	0.44
1:A:939:GLU:HG3	1:A:940:GLU:N	2.32	0.44
1:A:353:THR:HB	8:A:4120:HOH:O	2.17	0.44
1:A:459:ALA:C	1:A:461:ARG:H	2.20	0.44
1:A:373:LEU:HD13	1:A:397:LEU:HG	1.99	0.44
1:A:1209:GLU:HB3	1:A:1227:TYR:OH	2.17	0.44
1:A:1314:THR:HG22	1:A:1315:LEU:HD12	2.00	0.44
1:A:70:VAL:HG22	1:A:71:ASN:H	1.83	0.44
1:A:1038:MET:N	1:A:1040:GLN:NE2	2.41	0.44
1:A:232:ARG:HH12	1:A:273:LEU:HD13	1.80	0.44
1:A:1268:SER:O	1:A:1271:PHE:N	2.51	0.44
1:A:27:LEU:HD21	1:A:41:LEU:HB2	2.00	0.44
1:A:743:TYR:O	1:A:829:ARG:NH2	2.35	0.44
1:A:931:ALA:HA	1:A:941:VAL:HG21	2.00	0.44
1:A:111:GLN:HG3	1:A:150:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HD13	1:A:315:ILE:C	2.38	0.44
1:A:351:ILE:HD11	1:A:364:PHE:CE2	2.53	0.44
1:A:592:TYR:CE2	1:A:793:ARG:HD2	2.53	0.44
1:A:644:ASN:O	1:A:653:THR:HA	2.18	0.43
1:A:768:ASN:HD21	1:A:771:LYS:HG3	1.83	0.43
1:A:55:ILE:HD12	1:A:68:PHE:CE1	2.52	0.43
1:A:783:PRO:HB2	1:A:785:ASN:HB2	2.01	0.43
1:A:695:ILE:N	1:A:695:ILE:HD13	2.33	0.43
1:A:293:PRO:HG2	1:A:294:GLU:H	1.83	0.43
1:A:980:ARG:NH1	1:A:1161:GLU:OE1	2.51	0.43
1:A:348:GLY:O	1:A:352:ILE:HG12	2.19	0.43
1:A:1310:ASP:OD2	1:A:1313:THR:HG23	2.18	0.43
1:A:81:HIS:CD2	1:A:226:LEU:HD11	2.52	0.43
1:A:403:LEU:HD11	1:A:406:ILE:CD1	2.49	0.43
1:A:472:GLN:HE22	1:A:484:SER:HB3	1.82	0.43
1:A:1088:GLN:HG2	1:A:1133:TYR:CG	2.54	0.43
1:A:530:ASP:O	1:A:532:GLU:N	2.52	0.43
1:A:741:HIS:HE1	1:A:838:GLY:HA2	1.83	0.43
1:A:666:ILE:CD1	1:A:807:VAL:HG22	2.48	0.43
1:A:314:GLU:C	1:A:316:ALA:H	2.22	0.43
1:A:134:THR:OG1	1:A:137:GLU:HG3	2.18	0.43
1:A:963:THR:HG21	1:A:1181:ASP:OD2	2.18	0.43
1:A:433:VAL:HA	1:A:456:GLY:O	2.18	0.43
1:A:1104:PHE:CD2	1:A:1119:ASP:HB3	2.53	0.43
1:A:1000:ILE:O	1:A:1000:ILE:HG23	2.18	0.43
1:A:1018:GLY:HA2	1:A:1131:GLY:O	2.19	0.43
1:A:333:LEU:HA	1:A:336:PHE:HB2	2.00	0.43
1:A:766:THR:CG2	1:A:767:GLN:H	2.32	0.43
1:A:1039:GLY:N	1:A:1040:GLN:HE21	2.17	0.43
1:A:839:ARG:HB2	1:A:911:PHE:CD1	2.53	0.43
1:A:782:VAL:HG23	1:A:783:PRO:O	2.19	0.43
1:A:477:TRP:HD1	1:A:523:LEU:HD23	1.84	0.43
1:A:443:PRO:O	1:A:445:THR:HG23	2.19	0.43
1:A:103:ARG:HE	1:A:200:PHE:HB3	1.84	0.42
1:A:473:LEU:O	1:A:474:SER:HB2	2.18	0.42
1:A:785:ASN:CB	1:A:786:ARG:HH11	2.32	0.42
1:A:417:PHE:CD2	1:A:418:SER:N	2.87	0.42
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.49	0.42
1:A:361:ASN:HB2	1:A:362:PRO:HD3	2.01	0.42
1:A:9:PHE:N	1:A:9:PHE:CD1	2.87	0.42
1:A:1300:THR:HB	1:A:1301:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:MET:CE	1:A:126:LEU:HD23	2.49	0.42
1:A:707:PHE:CD1	1:A:899:ARG:NE	2.86	0.42
1:A:1104:PHE:HZ	1:A:1125:VAL:HG21	1.84	0.42
1:A:1007:ILE:O	1:A:1008:SER:CB	2.67	0.42
1:A:695:ILE:O	1:A:903:THR:HB	2.19	0.42
1:A:482:LEU:O	1:A:482:LEU:HD23	2.19	0.42
1:A:726:ALA:HB1	1:A:728:ASN:O	2.19	0.42
1:A:699:GLN:HE21	1:A:703:ASN:ND2	2.18	0.42
1:A:978:LEU:O	1:A:981:LYS:HB2	2.19	0.42
1:A:622:THR:CG2	1:A:622:THR:O	2.68	0.42
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.89	0.42
1:A:359:ASP:OD2	1:A:359:ASP:N	2.52	0.42
1:A:752:VAL:CG1	1:A:752:VAL:O	2.67	0.42
1:A:730:VAL:O	1:A:847:LYS:HA	2.19	0.42
1:A:1203:LEU:CD1	1:A:1203:LEU:C	2.87	0.42
1:A:1104:PHE:CZ	1:A:1125:VAL:HG21	2.54	0.42
1:A:324:GLU:OE2	1:A:327:ARG:NH2	2.53	0.42
1:A:233:VAL:HG22	1:A:273:LEU:HD11	2.00	0.42
1:A:1210:GLU:HG2	1:A:1212:HIS:NE2	2.35	0.42
1:A:98:HIS:ND1	1:A:99:PRO:CD	2.83	0.42
1:A:1077:THR:HG23	1:A:1082:SER:OG	2.20	0.42
1:A:116:THR:O	1:A:120:VAL:HG23	2.20	0.42
1:A:307:VAL:HG21	1:A:347:ILE:CG2	2.49	0.42
1:A:214:GLU:HG2	1:A:217:ARG:HH21	1.85	0.42
1:A:482:LEU:HD12	1:A:519:TYR:CD2	2.54	0.42
1:A:591:VAL:HG13	1:A:595:ASP:HB2	2.02	0.42
1:A:728:ASN:O	1:A:729:VAL:HG23	2.20	0.42
1:A:102:GLU:OE2	1:A:106:ARG:NH2	2.53	0.41
1:A:1046:MET:SD	1:A:1087:GLY:HA2	2.60	0.41
1:A:940:GLU:O	1:A:944:LYS:HG3	2.20	0.41
1:A:730:VAL:HG23	1:A:850:PHE:HE2	1.83	0.41
1:A:740:GLU:HG2	1:A:833:MET:CE	2.50	0.41
1:A:312:ALA:HB2	1:A:330:MET:HE1	2.02	0.41
1:A:626:LYS:HA	1:A:631:PHE:CD2	2.55	0.41
1:A:1045:LYS:O	1:A:1049:VAL:HG23	2.21	0.41
1:A:886:ASP:O	1:A:887:ASN:C	2.58	0.41
1:A:242:GLU:O	1:A:246:ASP:HB2	2.20	0.41
1:A:397:LEU:HD12	1:A:397:LEU:N	2.35	0.41
1:A:733:GLU:O	1:A:1294:GLN:NE2	2.49	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.86	0.41
1:A:504:VAL:HG23	1:A:505:GLU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.55	0.41
1:A:850:PHE:N	1:A:850:PHE:CD2	2.88	0.41
1:A:283:ILE:HA	1:A:284:PRO:HD3	1.87	0.41
1:A:1068:THR:HG22	8:A:4080:HOH:O	2.21	0.41
1:A:1173:ASN:HD22	1:A:1270:ILE:CD1	2.32	0.41
1:A:883:PHE:HZ	1:A:1140:TYR:CD2	2.39	0.41
1:A:964:LEU:N	1:A:965:PRO:CD	2.82	0.41
1:A:765:SER:OG	1:A:794:MET:HG2	2.20	0.41
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.02	0.41
1:A:980:ARG:O	1:A:984:VAL:HG23	2.20	0.41
1:A:768:ASN:ND2	1:A:771:LYS:HB2	2.35	0.41
1:A:614:HIS:CB	1:A:904:ASN:ND2	2.80	0.41
1:A:248:LYS:HD3	1:A:256:LEU:HD21	2.02	0.41
1:A:257:VAL:O	1:A:279:CYS:HA	2.21	0.41
1:A:538:LEU:HD12	1:A:539:ASP:H	1.86	0.41
1:A:1020:LEU:HB3	1:A:1032:THR:HG22	2.03	0.41
1:A:470:PRO:C	1:A:472:GLN:N	2.75	0.41
1:A:421:LYS:HG3	1:A:434:THR:CG2	2.51	0.41
1:A:1298:PRO:HG2	1:A:1300:THR:HG23	2.02	0.41
1:A:900:ILE:N	1:A:900:ILE:HD12	2.36	0.41
1:A:371:LEU:HD11	1:A:384:MET:HE2	2.02	0.41
1:A:1033:HIS:HD2	1:A:1035:GLY:N	2.19	0.41
1:A:218:LEU:C	1:A:220:ASP:N	2.73	0.41
1:A:123:MET:HE1	1:A:126:LEU:HD23	2.04	0.40
1:A:972:ILE:CG1	1:A:973:ALA:N	2.84	0.40
1:A:296:ILE:HD11	1:A:314:GLU:HG3	2.03	0.40
1:A:1011:LEU:HD12	1:A:1012:PRO:HD2	2.03	0.40
1:A:1250:LYS:HG3	1:A:1250:LYS:H	1.68	0.40
1:A:431:ALA:CB	1:A:434:THR:HG23	2.51	0.40
1:A:69:SER:N	1:A:125:THR:HG21	2.36	0.40
1:A:924:GLU:OE1	1:A:924:GLU:HA	2.20	0.40
1:A:73:CYS:SG	1:A:74:LEU:HG	2.61	0.40
1:A:839:ARG:HG2	1:A:840:HIS:N	2.36	0.40
1:A:788:VAL:HG21	1:A:1069:ASN:OD1	2.22	0.40
1:A:1235:ILE:O	1:A:1236:PRO:C	2.59	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	1291/1331 (97%)	1142 (88%)	117 (9%)	32 (2%)	7	12

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	602	GLU
1	A	1008	SER
1	A	1325	LYS
1	A	152	TYR
1	A	212	PRO
1	A	428	ASP
1	A	551	LYS
1	A	567	GLN
1	A	1253	ILE
1	A	1316	CYS
1	A	62	GLN
1	A	390	PRO
1	A	471	LYS
1	A	531	LEU
1	A	739	GLN
1	A	797	GLY
1	A	912	ARG
1	A	1288	ASN
1	A	552	ASP
1	A	1251	ARG
1	A	662	CYS
1	A	977	TYR
1	A	366	ALA
1	A	386	HIS
1	A	593	CYS
1	A	1002	PRO
1	A	1259	VAL

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Mol	Chain	Res	Type
1	A	258	VAL
1	A	1286	GLY
1	A	729	VAL
1	A	1329	VAL

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	1095/1123 (98%)	1052 (96%)	43 (4%)	39 68

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	219	LYS
1	A	224	LYS
1	A	246	ASP
1	A	253	ASP
1	A	255	LYS
1	A	256	LEU
1	A	306	LEU
1	A	315	ILE
1	A	378	THR
1	A	398	ARG
1	A	413	GLU
1	A	434	THR
1	A	480	GLU
1	A	494	GLN
1	A	530	ASP
1	A	624	GLU
1	A	646	THR
1	A	662	CYS
1	A	743	TYR
1	A	761	GLU
1	A	798	PHE

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Mol	Chain	Res	Type
1	A	807	VAL
1	A	821	ARG
1	A	826	MET
1	A	909	THR
1	A	911	PHE
1	A	939	GLU
1	A	983	GLU
1	A	1002	PRO
1	A	1013	PHE
1	A	1040	GLN
1	A	1072	PRO
1	A	1084	ASP
1	A	1085	LEU
1	A	1119	ASP
1	A	1143	GLU
1	A	1203	LEU
1	A	1239	PHE
1	A	1250	LYS
1	A	1253	ILE
1	A	1268	SER
1	A	1311	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	143	GLN
1	A	223	GLN
1	A	250	GLN
1	A	332	GLN
1	A	449	GLN
1	A	472	GLN
1	A	478	ASN
1	A	483	GLN
1	A	556	ASN
1	A	558	GLN
1	A	567	GLN
1	A	585	GLN
1	A	642	ASN
1	A	699	GLN
1	A	703	ASN
1	A	768	ASN

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Mol	Chain	Res	Type
1	A	817	HIS
1	A	893	ASN
1	A	904	ASN
1	A	956	ASN
1	A	1033	HIS
1	A	1040	GLN
1	A	1048	GLN
1	A	1086	ASN
1	A	1173	ASN
1	A	1288	ASN
1	A	1311	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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	PO4	A	2001	-	4,4,4	1.14	0	6,6,6	0.27	0
2	PO4	A	2002	-	4,4,4	1.12	0	6,6,6	0.27	0
2	PO4	A	2003	-	4,4,4	1.20	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACY	A	3001	-	1,3,3	1.89	0	0,3,3	0.00	-
4	FES	A	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	4003	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	A	4004	-	48,58,58	2.80	17 (35%)	54,89,89	3.14	19 (35%)
6	SAL	A	4005	-	7,10,10	1.91	3 (42%)	10,13,13	1.19	0

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	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2003	-	-	0/0/0/0	0/0/0/0
7	ACY	A	3001	-	-	0/0/0/0	0/0/0/0
4	FES	A	4002	1	-	0/0/4/4	0/1/1/1
4	FES	A	4003	1	-	0/0/4/4	0/1/1/1
5	FAD	A	4004	-	-	0/30/50/50	0/6/6/6
6	SAL	A	4005	-	-	0/0/4/4	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4005	SAL	C3-C2	2.31	1.43	1.39
6	A	4005	SAL	C6-C1	2.59	1.44	1.39
5	A	4004	FAD	C5A-C4A	2.63	1.46	1.40
5	A	4004	FAD	C10-N1	2.89	1.40	1.35
5	A	4004	FAD	O4B-C4B	2.94	1.51	1.45
5	A	4004	FAD	C9-C9A	2.95	1.47	1.40
5	A	4004	FAD	C6-C5X	2.96	1.46	1.41
6	A	4005	SAL	C5-C6	3.10	1.45	1.38
5	A	4004	FAD	C4X-N5	3.33	1.38	1.33
5	A	4004	FAD	C8-C7	3.51	1.50	1.41
5	A	4004	FAD	C4-C4X	3.52	1.48	1.41
5	A	4004	FAD	C9A-C5X	3.74	1.50	1.42
5	A	4004	FAD	C2A-N1A	3.84	1.41	1.33
5	A	4004	FAD	C2A-N3A	4.13	1.39	1.32
5	A	4004	FAD	C5X-N5	4.21	1.42	1.35
5	A	4004	FAD	C4A-N3A	4.82	1.42	1.35
5	A	4004	FAD	C4-N3	5.25	1.42	1.33
5	A	4004	FAD	C4X-C10	5.52	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4004	FAD	O4B-C1B	8.04	1.51	1.41
5	A	4004	FAD	C9A-N10	8.42	1.50	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4004	FAD	N3A-C2A-N1A	-9.98	121.25	128.89
5	A	4004	FAD	C4-C4X-C10	-7.88	114.90	119.94
5	A	4004	FAD	C5X-C9A-N10	-7.57	111.87	117.62
5	A	4004	FAD	C4X-C10-N10	-5.51	117.28	120.52
5	A	4004	FAD	O4B-C1B-N9A	-4.24	99.22	108.10
5	A	4004	FAD	C4X-C4-N3	-3.84	118.33	123.59
5	A	4004	FAD	O3B-C3B-C4B	-2.59	103.30	111.05
5	A	4004	FAD	C8M-C8-C9	-2.44	113.65	120.28
5	A	4004	FAD	C1'-N10-C9A	-2.14	116.46	118.86
5	A	4004	FAD	O4B-C4B-C5B	-2.09	101.85	109.32
5	A	4004	FAD	P-O3P-PA	2.02	138.41	132.73
5	A	4004	FAD	C2B-C1B-N9A	2.06	117.44	114.29
5	A	4004	FAD	O2'-C2'-C3'	2.07	114.23	109.02
5	A	4004	FAD	O3'-C3'-C4'	2.24	114.40	108.75
5	A	4004	FAD	C4A-C5A-N7A	2.68	111.94	109.48
5	A	4004	FAD	C8M-C8-C7	3.40	128.21	120.73
5	A	4004	FAD	C4X-N5-C5X	4.38	121.80	116.76
5	A	4004	FAD	C4-C4X-N5	5.52	125.42	118.72
5	A	4004	FAD	C4-N3-C2	10.62	124.42	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4002	FES	2	0
4	A	4003	FES	1	0
5	A	4004	FAD	3	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, 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	1297/1331 (97%)	-0.29	30 (2%) 64 57	9, 35, 61, 88	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1324	SER	7.1
1	A	1318	THR	5.4
1	A	1325	LYS	4.7
1	A	1326	SER	4.6
1	A	1289	ALA	4.3
1	A	3	ALA	4.2
1	A	61	LEU	4.2
1	A	1317	VAL	4.1
1	A	533	ASP	3.7
1	A	1107	LYS	3.2
1	A	1328	SER	3.0
1	A	1286	GLY	3.0
1	A	530	ASP	3.0
1	A	1327	TRP	2.8
1	A	566	ASP	2.8
1	A	1290	LYS	2.8
1	A	1331	ILE	2.8
1	A	292	GLY	2.5
1	A	220	ASP	2.5
1	A	398	ARG	2.5
1	A	1287	ASP	2.4
1	A	1291	GLN	2.4
1	A	534	MET	2.4
1	A	1288	ASN	2.3
1	A	1143	GLU	2.2
1	A	717	GLY	2.2
1	A	272	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1329	VAL	2.2
1	A	391	GLY	2.1
1	A	192	PRO	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(Å ²)	Q<0.9
7	ACY	A	3001	4/4	0.90	0.22	4.41	55,55,56,56	0
6	SAL	A	4005	10/10	0.87	0.20	3.26	31,33,42,42	0
5	FAD	A	4004	53/53	0.96	0.15	0.54	25,36,44,45	0
2	PO4	A	2001	5/5	0.98	0.11	-0.11	41,42,44,45	0
2	PO4	A	2002	5/5	0.96	0.12	-1.25	68,68,69,70	0
4	FES	A	4003	4/4	0.98	0.09	-1.30	22,23,23,26	0
3	CA	A	4001	1/1	0.96	0.06	-3.74	28,28,28,28	0
4	FES	A	4002	4/4	0.98	0.05	-4.07	31,31,34,36	0
2	PO4	A	2003	5/5	0.96	0.12	-	70,70,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.