



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 PM GMT

PDB ID : 4IU8
Title : Crystal structure of a membrane transporter (selenomethionine derivative)
Authors : Yan, H.; Huang, W.; Yan, C.; Gong, X.; Jiang, S.; Zhao, Y.; Wang, J.; Shi, Y.
Deposited on : 2013-01-20
Resolution : 3.11 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

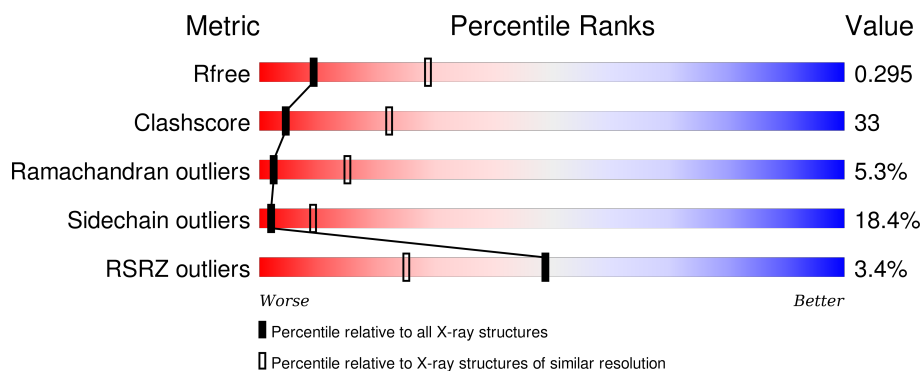
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	468	
1	B	468	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NO3	A	501	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6214 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.

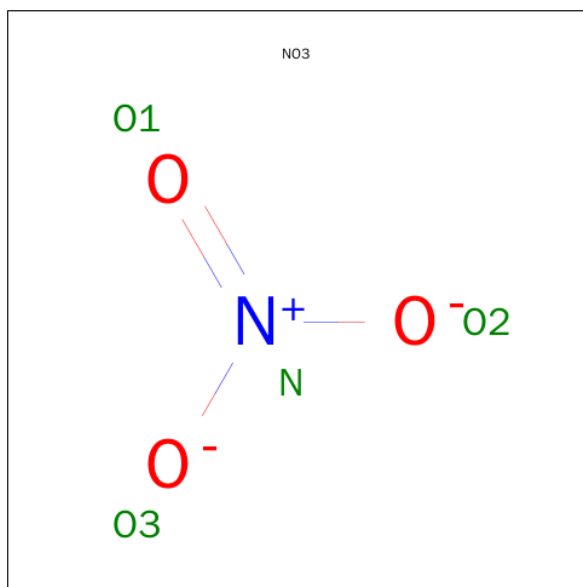
- Molecule 1 is a protein called Nitrite extrusion protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	Se	0	0	0
			3081	2059	490	514	5	13			
1	B	427	Total	C	N	O	S	Se	0	0	0
			3129	2092	500	519	5	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	LEU	-	EXPRESSION TAG	UNP P37758
A	464	GLU	-	EXPRESSION TAG	UNP P37758
A	465	VAL	-	EXPRESSION TAG	UNP P37758
A	466	LEU	-	EXPRESSION TAG	UNP P37758
A	467	PHE	-	EXPRESSION TAG	UNP P37758
A	468	GLN	-	EXPRESSION TAG	UNP P37758
B	463	LEU	-	EXPRESSION TAG	UNP P37758
B	464	GLU	-	EXPRESSION TAG	UNP P37758
B	465	VAL	-	EXPRESSION TAG	UNP P37758
B	466	LEU	-	EXPRESSION TAG	UNP P37758
B	467	PHE	-	EXPRESSION TAG	UNP P37758
B	468	GLN	-	EXPRESSION TAG	UNP P37758

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		

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.

Chain A:

Sequence logo for Chain A, showing amino acid conservation across 100 positions. The y-axis represents information content in bits, ranging from 0 to 2.0. The x-axis shows positions 1 to 100. A color scale at the top indicates the percentage of conservation: 2% (red), 41% (green), 38% (orange), 11% (yellow), and 10% (grey).

Key amino acids and their approximate conservation percentages (from top to bottom):

- Position 1: MSE (2%)
- Position 2: ALA (41%)
- Position 3: LEU (41%)
- Position 4: GLN (41%)
- Position 5: ASN (41%)
- Position 6: GLU (41%)
- Position 7: LYS (41%)
- Position 8: SER (41%)
- Position 9: ARG (41%)
- Position 10: TYR (41%)
- Position 11: L12 (41%)
- Position 12: L13 (41%)
- Position 13: R14 (41%)
- Position 14: D15 (41%)
- Position 15: W16 (41%)
- Position 16: E19 (41%)
- Position 17: R20 (41%)
- Position 18: P21 (41%)
- Position 19: A22 (41%)
- Position 20: F23 (41%)
- Position 21: W24 (41%)
- Position 22: K27 (41%)
- Position 23: R29 (41%)
- Position 24: K29 (41%)
- Position 25: F30 (41%)
- Position 26: R34 (41%)
- Position 27: R35 (41%)
- Position 28: L36 (41%)
- Position 29: W37 (41%)
- Position 30: I38 (41%)
- Position 31: S39 (41%)
- Position 32: V40 (41%)
- Position 33: S41 (41%)
- Position 34: C42 (41%)
- Position 35: L43 (41%)
- Position 36: L44 (41%)
- Position 37: L45 (41%)
- Position 38: L46 (41%)
- Position 39: F47 (41%)
- Position 40: C48 (41%)
- Position 41: V49 (41%)
- Position 42: W50 (41%)
- Position 43: W51 (41%)
- Position 44: L52 (41%)
- Position 45: F53 (41%)
- Position 46: S54 (41%)
- Position 47: T57 (41%)
- Position 48: V58 (41%)
- Position 49: W59 (41%)
- Position 50: L60 (41%)
- Position 51: N61 (41%)
- Position 52: R62 (41%)
- Position 53: L63 (41%)
- Position 54: G64 (41%)
- Position 55: R65 (41%)
- Position 56: M66 (41%)
- Position 57: F67 (41%)
- Position 58: T68 (41%)
- Position 59: T69 (41%)
- Position 60: D70 (41%)
- Position 61: Q71 (41%)
- Position 62: L72 (41%)
- Position 63: F73 (41%)
- Position 64: L74 (41%)
- Position 65: L75 (41%)
- Position 66: T76 (41%)
- Position 67: A77 (41%)
- Position 68: L78 (41%)
- Position 69: P79 (41%)
- Position 70: G83 (41%)
- Position 71: R87 (41%)
- Position 72: V88 (41%)
- Position 73: P89 (41%)
- Position 74: Y90 (41%)
- Position 75: S91 (41%)
- Position 76: F92 (41%)
- Position 77: M93 (41%)
- Position 78: V94 (41%)
- Position 79: P95 (41%)
- Position 80: I96 (41%)
- Position 81: F97 (41%)
- Position 82: G98 (41%)
- Position 83: G99 (41%)
- Position 84: R100 (41%)
- Position 85: R101 (41%)
- Position 86: W102 (41%)
- Position 87: T103 (41%)
- Position 88: V104 (41%)
- Position 89: T107 (41%)
- Position 90: A108 (41%)
- Position 91: I109 (41%)
- Position 92: L110 (41%)
- Position 93: I111 (41%)
- Position 94: I112 (41%)
- Position 95: P113 (41%)
- Position 96: C114 (41%)
- Position 97: V115 (41%)
- Position 98: I119 (41%)
- Position 99: Q122 (41%)
- Position 100: N123 (41%)
- Position 101: P124 (41%)
- Position 102: T125 (41%)
- Position 103: T126 (41%)
- Position 104: P127 (41%)
- Position 105: F128 (41%)
- Position 106: I132 (41%)
- Position 107: A135 (41%)
- Position 108: F136 (41%)
- Position 109: L137 (41%)
- Position 110: A143 (41%)
- Position 111: N144 (41%)
- Position 112: F145 (41%)
- Position 113: G231 (41%)
- Position 114: M232 (41%)
- Position 115: N233 (41%)
- Position 116: D234 (41%)
- Position 117: I235 (41%)
- Position 118: A236 (41%)
- Position 119: S148 (41%)
- Position 120: M149 (41%)
- Position 121: A150 (41%)
- Position 122: N151 (41%)
- Position 123: F154 (41%)
- Position 124: F155 (41%)
- Position 125: P156 (41%)
- Position 126: P157 (41%)
- Position 127: K160 (41%)
- Position 128: S163 (41%)
- Position 129: P169 (41%)
- Position 130: G170 (41%)
- Position 131: L171 (41%)
- Position 132: G172 (41%)
- Position 133: M173 (41%)
- Position 134: L174 (41%)
- Position 135: G175 (41%)
- Position 136: V176 (41%)
- Position 137: S177 (41%)
- Position 138: V178 (41%)
- Position 139: M179 (41%)
- Position 140: Q180 (41%)
- Position 141: L181 (41%)
- Position 142: F185 (41%)
- Position 143: G270 (41%)
- Position 144: F271 (41%)
- Position 145: S272 (41%)
- Position 146: F275 (41%)
- Position 147: A276 (41%)
- Position 148: M277 (41%)
- Position 149: L278 (41%)
- Position 150: A279 (41%)
- Position 151: K280 (41%)
- Position 152: D285 (41%)
- Position 153: V286 (41%)
- Position 154: R287 (41%)
- Position 155: L288 (41%)
- Position 156: L289 (41%)
- Position 157: F293 (41%)
- Position 158: P296 (41%)
- Position 159: F297 (41%)
- Position 160: I298 (41%)
- Position 161: A302 (41%)
- Position 162: R303 (41%)
- Position 163: V316 (41%)
- Position 164: R317 (41%)
- Position 165: V318 (41%)
- Position 166: T319 (41%)
- Position 167: L320 (41%)
- Position 168: I321 (41%)
- Position 169: N322 (41%)
- Position 170: F323 (41%)
- Position 171: I324 (41%)
- Position 172: F325 (41%)
- Position 173: V326 (41%)
- Position 174: A327 (41%)
- Position 175: L328 (41%)
- Position 176: F329 (41%)
- Position 177: S330 (41%)
- Position 178: A331 (41%)
- Position 179: L332 (41%)
- Position 180: F333 (41%)
- Position 181: F334 (41%)
- Position 182: L335 (41%)
- Position 183: T336 (41%)
- Position 184: L337 (41%)
- Position 185: P338 (41%)
- Position 186: G339 (41%)
- Position 187: T340 (41%)
- Position 188: G341 (41%)
- Position 189: S342 (41%)
- Position 190: G343 (41%)
- Position 191: N344 (41%)
- Position 192: F345 (41%)
- Position 193: V351 (41%)
- Position 194: F352 (41%)
- Position 195: R353 (41%)
- Position 196: G354 (41%)
- Position 197: L355 (41%)
- Position 198: T358 (41%)
- Position 199: A359 (41%)
- Position 200: L360 (41%)
- Position 201: L361 (41%)
- Position 202: G362 (41%)
- Position 203: S363 (41%)
- Position 204: T366 (41%)
- Position 205: F367 (41%)
- Position 206: I370 (41%)
- Position 207: T374 (41%)
- Position 208: R375 (41%)
- Position 209: Q376 (41%)
- Position 210: I377 (41%)
- Position 211: T378 (41%)
- Position 212: L379 (41%)
- Position 213: R380 (41%)
- Position 214: R381 (41%)
- Position 215: K

Chain B:

4%

39%

43%

9%

9%

MSE

ALA

LEU

GLN

ASN

GLY

LYS

ASN

SER

ARG

TYR

L12

L13

R14

D15

R20

R26

F29

A32

R33

R34

R35

R36

R37

I38

S39

V40

L43

L44

L45

C48

R51

L52

F53

S54

A55

V56

T57

V58

N59

L60

R61

K62

I63

L64

G65

R66

F67

D70

Q71

L72

F73

L74

L75

T76

A77

L78

F79

S80

V81

S82

G83

A84

L85

V88

P88

F89

F92

R93

R100

R101

W102

T103

V104

F105

I109

L110

I111

I112

P113

C114

V115

W116

L117

V121

Q122

N123

P124

W125

T126

F127

F128

G129

I130

F131

I132

V133

I134

A135

L136

G139

F140

A141

G142

A143

N144

F145

S148

M149

G150

M151

I152

S153

F154

F155

F156

K160

S163

A164

L165

G166

I167

M168

L171

G172

M173

L174

G175

V176

S177

V178

M179

Q180

L181

A183

P184

L185

L186

I187

F188

V189

F192

A193

F194

L195

M198

P201

Q202

A203

D204

G205

S206

V207

M208

S209

L210

A211

N212

M427	M428	T429	G430	S431	P432	V433	G434	A435	M436	K437	L440	I441	V445	C446	V447	L448	L449	T450	V453	V454	GLY	ARG	ARG	LYS	PHE	SER	GLN	LYS	LEU	GLU	VAL	LEU	PHE	GLN																			
A359	G360	L361	G362	S363	T366	F367	Q368	M369	I370	A371	V372	I373	F374	R375	Q376	I377	T378	I379	T380	R381	VAL	LYS	MSE	LYS	GLY	GLY	ASP	GLU	GLN	A392	H393	K394	E395	A401	A402	A403	L404	G405	F406	I407	I410	V413	G414	G415	F416	F417	I418	P419	Q420	A421	F422	S425	L426
R290	L291	A292	F293	F294	G295	P296	F297	I298	G299	A300	I301	A302	R303	S304	V305	I309	S310	F313	G314	G315	V318	T319	L320	F323	I324	F325	M326	F329	S330	A331	L332	L333	F334	L335	T336	L337	P338	G339	T340	G341	S342	G343	N344	F345	F348	Y349	F352	M353	F356	I357	T358		
W215	I216	W217	V218	P219	L220	L221	A222	T225	A228	W229	S230	G231	M232	I235	ALA	SER	SER	ARG	ALA	SER	I242	A243	D244	P247	L252	W255	L256	L257	S258	L259	L262	A263	T264	F265	G266	S267	F268	I269	G270	F271	S272	A273	A276	W277	L278	A279	Q282	I288	L289				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.58Å 117.50Å 127.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.11 40.03 – 3.11	Depositor EDS
% Data completeness (in resolution range)	82.7 (40.00-3.11) 82.9 (40.03-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.299 0.240 , 0.295	Depositor DCC
R_{free} test set	1222 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	1.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 24412 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6214	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: NO3

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	0.67	5/3150 (0.2%)	0.79	3/4276 (0.1%)
1	B	0.71	3/3202 (0.1%)	0.83	4/4349 (0.1%)
All	All	0.69	8/6352 (0.1%)	0.81	7/8625 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	TRP	CD2-CE2	7.37	1.50	1.41
1	B	215	TRP	CD2-CE2	6.32	1.49	1.41
1	A	229	TRP	CD2-CE2	5.53	1.48	1.41
1	A	451	TRP	CD2-CE2	5.34	1.47	1.41
1	A	50	TRP	CD2-CE2	5.20	1.47	1.41
1	A	37	TRP	CD2-CE2	5.11	1.47	1.41
1	B	255	TRP	CD2-CE2	5.08	1.47	1.41
1	B	37	TRP	CD2-CE2	5.08	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	MSE	CG-SE-CE	6.04	112.19	98.90
1	A	52	LEU	CA-CB-CG	6.02	129.14	115.30
1	B	277	MSE	CA-CB-CG	-5.87	103.32	113.30
1	B	247	PRO	N-CA-CB	5.84	110.31	103.30
1	B	33	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	93	MSE	CA-CB-CG	-5.16	104.52	113.30
1	A	289	LEU	CA-CB-CG	5.03	126.86	115.30

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	3081	0	3049	207	0
1	B	3129	0	3092	197	0
2	A	4	0	0	1	0
All	All	6214	0	6141	402	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 33.

All (402) 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:123:ASN:O	1:A:126:THR:HG22	1.47	1.11
1:B:12:LEU:HD23	1:B:13:LEU:H	1.12	1.08
1:A:63:ILE:HG22	1:A:64:GLY:H	1.23	1.03
1:A:88:VAL:HB	1:A:89:PRO:HD3	1.41	1.01
1:B:93:MSE:HG2	1:B:102:TRP:CH2	1.96	1.00
1:B:74:LEU:HD23	1:B:420:GLN:HE22	1.24	0.98
1:A:269:ILE:HD12	1:A:415:GLY:HA3	1.50	0.94
1:B:123:ASN:O	1:B:126:THR:HB	1.68	0.94
1:A:320:LEU:HD11	1:A:450:THR:HB	1.52	0.91
1:A:374:PHE:HE2	1:A:399:GLU:HG3	1.35	0.90
1:A:323:PHE:CE1	1:A:446:CYS:HB3	2.05	0.90
1:B:12:LEU:HD23	1:B:13:LEU:N	1.86	0.89
1:A:324:ILE:HG12	1:A:447:VAL:HG13	1.54	0.88
1:A:324:ILE:HG12	1:A:447:VAL:CG1	2.04	0.87
1:B:258:SER:HB3	1:B:407:ILE:HG12	1.57	0.87
1:A:44:LEU:HD21	1:A:178:VAL:HG11	1.57	0.86
1:B:74:LEU:HD23	1:B:420:GLN:NE2	1.89	0.86
1:A:64:GLY:HA3	1:A:124:PRO:HB3	1.58	0.83
1:A:374:PHE:CE2	1:A:399:GLU:HG3	2.15	0.81
1:B:100:ARG:HG3	1:B:232:MSE:HB3	1.63	0.81
1:A:433:VAL:H	1:A:436:MSE:HG3	1.46	0.80
1:A:323:PHE:CD1	1:A:446:CYS:HB3	2.17	0.80
1:A:93:MSE:HG2	1:A:102:TRP:CH2	2.18	0.79
1:B:63:ILE:HG22	1:B:64:GLY:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ALA:HB3	1:A:288:ILE:HD13	1.64	0.78
1:A:53:PHE:O	1:A:57:THR:OG1	2.03	0.77
1:A:111:ILE:HG23	1:A:218:VAL:HG22	1.65	0.77
1:A:73:PHE:CZ	1:A:277:MSE:HB3	2.20	0.77
1:B:276:ALA:HA	1:B:288:ILE:HD12	1.66	0.77
1:A:279:ALA:CB	1:A:288:ILE:HD13	2.15	0.76
1:B:320:LEU:HD23	1:B:450:THR:HB	1.65	0.76
1:B:300:ALA:O	1:B:303:ARG:HB3	1.86	0.76
1:B:51:MSE:HE3	1:B:51:MSE:HA	1.69	0.75
1:A:88:VAL:HB	1:A:89:PRO:CD	2.16	0.74
1:A:52:LEU:HD23	1:A:179:MSE:HE1	1.69	0.74
1:B:82:SER:CB	1:B:139:GLY:HA3	2.18	0.74
1:A:304:SER:O	1:A:306:GLY:N	2.20	0.74
1:A:77:ALA:HB2	1:A:419:PRO:HB2	1.69	0.73
1:A:123:ASN:O	1:A:126:THR:CG2	2.32	0.73
1:A:396:ALA:HA	1:A:399:GLU:HB3	1.71	0.72
1:B:426:LEU:O	1:B:430:GLY:HA2	1.89	0.72
1:B:65:PHE:CD1	1:B:67:PHE:CE2	2.77	0.72
1:B:35:ASN:HD21	1:B:232:MSE:HA	1.53	0.72
1:A:145:PHE:O	1:A:149:MSE:HB2	1.89	0.71
1:B:363:SER:O	1:B:366:THR:HG22	1.90	0.71
1:B:81:VAL:O	1:B:85:LEU:HB2	1.91	0.71
1:A:320:LEU:O	1:A:324:ILE:HG13	1.91	0.70
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.73	0.70
1:A:94:VAL:O	1:A:98:GLY:N	2.22	0.70
1:B:93:MSE:HG2	1:B:102:TRP:CZ3	2.27	0.69
1:A:72:LEU:O	1:A:76:THR:HG23	1.92	0.69
1:A:323:PHE:HB3	1:A:447:VAL:HG22	1.72	0.69
1:B:82:SER:HB2	1:B:139:GLY:HA3	1.74	0.69
1:B:278:LEU:HD22	1:B:422:PHE:CZ	2.28	0.69
1:A:35:ASN:OD1	1:A:232:MSE:HA	1.93	0.68
1:B:258:SER:CB	1:B:407:ILE:HG12	2.23	0.68
1:B:330:SER:OG	1:B:440:LEU:HD23	1.94	0.68
1:B:71:GLN:HB2	1:B:128:PHE:CE2	2.29	0.67
1:A:24:TRP:NE1	1:A:29:LYS:HB3	2.10	0.67
1:A:103:THR:HG21	1:A:232:MSE:SE	2.44	0.67
1:A:63:ILE:HG22	1:A:64:GLY:N	2.03	0.67
1:B:425:SER:OG	1:B:432:PRO:HA	1.93	0.67
1:A:111:ILE:HG12	1:A:221:LEU:HD23	1.76	0.67
1:B:67:PHE:CE1	1:B:128:PHE:HD2	2.11	0.67
1:B:367:PHE:C	1:B:369:MSE:H	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HG21	1:A:407:ILE:HD13	1.75	0.67
1:A:433:VAL:N	1:A:436:MSE:HG3	2.10	0.67
1:A:65:PHE:HE1	1:A:126:THR:HG23	1.59	0.67
1:B:12:LEU:CD2	1:B:13:LEU:H	2.00	0.66
1:A:425:SER:OG	1:A:432:PRO:O	2.12	0.66
1:A:65:PHE:HB3	1:A:67:PHE:CE2	2.31	0.66
1:A:323:PHE:HE1	1:A:446:CYS:HB3	1.58	0.66
1:A:304:SER:C	1:A:306:GLY:H	1.99	0.65
1:A:363:SER:O	1:A:367:PHE:HB2	1.96	0.65
1:B:302:ALA:HA	1:B:305:VAL:HB	1.79	0.64
1:A:443:TYR:O	1:A:447:VAL:HG23	1.97	0.64
1:B:324:ILE:HD13	1:B:447:VAL:HG21	1.78	0.64
1:B:35:ASN:ND2	1:B:232:MSE:HA	2.13	0.64
1:A:45:LEU:O	1:A:48:CYS:HB2	1.97	0.64
1:A:271:PHE:CE1	1:A:418:ILE:HD13	2.32	0.64
1:A:149:MSE:HE1	1:A:169:GLY:CA	2.28	0.64
1:A:230:SER:O	1:A:232:MSE:N	2.30	0.64
1:A:61:ASN:OD1	1:A:66:ASN:HA	1.98	0.64
1:B:258:SER:HA	1:B:407:ILE:HG23	1.78	0.63
1:B:71:GLN:HB2	1:B:128:PHE:CZ	2.33	0.63
1:B:67:PHE:CD1	1:B:128:PHE:HD2	2.16	0.63
1:B:323:PHE:CE1	1:B:446:CYS:HB3	2.33	0.63
1:B:65:PHE:CD1	1:B:67:PHE:HE2	2.15	0.63
1:B:51:MSE:HA	1:B:51:MSE:CE	2.26	0.62
1:B:100:ARG:HD3	1:B:232:MSE:O	1.99	0.62
1:B:426:LEU:HD21	1:B:432:PRO:HG3	1.80	0.62
1:B:349:TYR:CE2	1:B:353:MSE:HE3	2.35	0.62
1:A:264:THR:OG1	1:A:362:GLY:HA3	1.99	0.62
1:A:43:LEU:HD21	1:A:144:ASN:O	2.00	0.61
1:B:29:LYS:O	1:B:33:ARG:HG2	2.00	0.61
1:B:32:ALA:HB1	1:B:156:PHE:CE2	2.35	0.61
1:B:122:GLN:HG2	1:B:198:ASN:HB2	1.83	0.61
1:B:297:PHE:CZ	1:B:301:ILE:HD11	2.35	0.60
1:B:51:MSE:O	1:B:53:PHE:N	2.31	0.60
1:B:425:SER:HG	1:B:432:PRO:HA	1.64	0.60
1:A:24:TRP:CE2	1:A:29:LYS:HB3	2.37	0.60
1:B:111:ILE:O	1:B:115:VAL:HG12	2.00	0.60
1:B:116:TRP:CH2	1:B:133:VAL:HG21	2.36	0.60
1:B:174:LEU:O	1:B:177:SER:HB3	2.02	0.60
1:A:262:LEU:C	1:A:262:LEU:HD23	2.22	0.60
1:A:59:ASN:HB3	1:A:208:MSE:CE	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:O	1:B:225:THR:HB	2.01	0.60
1:B:149:MSE:HE3	1:B:165:LEU:HB3	1.83	0.60
1:B:181:LEU:O	1:B:185:LEU:HD22	2.01	0.59
1:B:184:PRO:HG3	1:B:289:LEU:HD13	1.84	0.59
1:B:326:MSE:HG2	1:B:358:THR:HB	1.84	0.59
1:A:323:PHE:CE1	1:A:446:CYS:CB	2.85	0.59
1:A:181:LEU:HD13	1:A:293:PHE:CE2	2.37	0.59
1:A:265:PHE:HB2	1:A:363:SER:HB3	1.84	0.59
1:B:302:ALA:O	1:B:361:LEU:HA	2.02	0.59
1:A:234:ASP:C	1:A:235:ILE:HG13	2.22	0.59
1:A:234:ASP:O	1:A:235:ILE:HG13	2.02	0.59
1:B:434:GLY:O	1:B:437:LYS:HB2	2.02	0.59
1:A:278:LEU:HD22	1:A:422:PHE:CZ	2.38	0.58
1:A:59:ASN:HB3	1:A:208:MSE:HE1	1.84	0.58
1:A:92:PHE:O	1:A:96:ILE:HG12	2.04	0.58
1:B:192:PHE:HB3	1:B:195:LEU:HD12	1.86	0.58
1:B:183:ALA:HB3	1:B:184:PRO:HD3	1.85	0.58
1:B:360:GLY:O	1:B:363:SER:HB3	2.03	0.57
1:A:324:ILE:HG12	1:A:447:VAL:HG11	1.84	0.57
1:A:38:ILE:HG21	1:A:232:MSE:HG3	1.85	0.57
1:A:176:VAL:O	1:A:179:MSE:HG3	2.04	0.57
1:B:154:PHE:HB3	1:B:235:ILE:HD11	1.85	0.57
1:B:325:PHE:O	1:B:329:PHE:CD2	2.58	0.57
1:A:271:PHE:O	1:A:275:PHE:HB2	2.05	0.56
1:B:105:PHE:CE2	1:B:109:ILE:HD11	2.41	0.56
1:B:305:VAL:O	1:B:309:ILE:HB	2.05	0.56
1:A:43:LEU:HD13	1:A:172:GLY:HA3	1.88	0.56
1:A:40:VAL:HG23	1:A:41:SER:N	2.21	0.56
1:B:279:ALA:HB3	1:B:288:ILE:CD1	2.36	0.56
1:A:107:THR:O	1:A:110:LEU:HB2	2.05	0.55
1:B:270:GLY:HA3	1:B:418:ILE:HD12	1.86	0.55
1:A:110:LEU:HB3	1:A:221:LEU:HD21	1.89	0.55
1:B:257:LEU:HD22	1:B:370:ILE:HG12	1.89	0.55
1:A:358:THR:C	1:A:360:GLY:H	2.09	0.55
1:B:324:ILE:HD13	1:B:447:VAL:CG2	2.37	0.55
1:B:263:ALA:O	1:B:326:MSE:HE1	2.07	0.55
1:B:33:ARG:O	1:B:37:TRP:CD1	2.60	0.55
1:B:76:THR:O	1:B:79:PRO:HD2	2.06	0.54
1:A:101:ARG:O	1:A:104:VAL:HG22	2.08	0.54
1:A:270:GLY:HA2	1:A:415:GLY:HA2	1.88	0.54
1:B:44:LEU:HA	1:B:172:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD13	1:B:134:ILE:HG21	1.88	0.54
1:B:216:ILE:O	1:B:219:PRO:HD2	2.07	0.54
1:A:333:LEU:HD23	1:A:436:MSE:HE1	1.89	0.54
1:A:72:LEU:HB3	1:A:277:MSE:HE2	1.88	0.54
1:A:269:ILE:HD12	1:A:415:GLY:CA	2.31	0.54
1:A:52:LEU:C	1:A:54:SER:H	2.12	0.54
1:A:52:LEU:HA	1:A:179:MSE:HE1	1.91	0.53
1:B:116:TRP:CZ3	1:B:133:VAL:CG2	2.90	0.53
1:B:335:LEU:HD12	1:B:335:LEU:H	1.74	0.53
1:B:128:PHE:CE1	1:B:132:ILE:HD11	2.42	0.53
1:B:401:ALA:HA	1:B:404:LEU:HD12	1.90	0.53
1:A:73:PHE:CE1	1:A:277:MSE:HB3	2.43	0.53
1:B:269:ILE:HG22	1:B:415:GLY:HA3	1.91	0.53
1:A:43:LEU:O	1:A:44:LEU:C	2.47	0.53
1:B:335:LEU:HD12	1:B:335:LEU:N	2.24	0.53
1:A:115:VAL:O	1:A:119:ILE:HG13	2.08	0.53
1:B:302:ALA:HB1	1:B:361:LEU:HB2	1.91	0.53
1:B:126:THR:HG22	1:B:131:PHE:HE2	1.73	0.53
1:B:63:ILE:HG22	1:B:64:GLY:N	2.22	0.53
1:B:276:ALA:O	1:B:288:ILE:HD11	2.07	0.53
1:B:184:PRO:CG	1:B:289:LEU:HD13	2.39	0.53
1:B:416:PHE:O	1:B:419:PRO:HD2	2.09	0.53
1:A:19:GLU:O	1:A:21:PRO:HD3	2.09	0.53
1:A:261:TYR:HA	1:A:264:THR:HG22	1.91	0.52
1:A:370:ILE:CG2	1:A:407:ILE:HD13	2.38	0.52
1:B:202:GLN:O	1:B:205:GLY:N	2.38	0.52
1:B:277:MSE:HA	1:B:277:MSE:CE	2.39	0.52
1:B:323:PHE:CD1	1:B:446:CYS:HB3	2.44	0.52
1:B:93:MSE:HG2	1:B:102:TRP:CZ2	2.43	0.52
1:A:333:LEU:HD23	1:A:436:MSE:CE	2.39	0.52
1:A:304:SER:C	1:A:306:GLY:N	2.59	0.52
1:A:63:ILE:CG2	1:A:64:GLY:H	2.05	0.52
1:A:279:ALA:HB3	1:A:288:ILE:CD1	2.37	0.52
1:A:52:LEU:HA	1:A:179:MSE:CE	2.40	0.52
1:A:265:PHE:HB2	1:A:363:SER:CB	2.40	0.52
1:B:323:PHE:HB3	1:B:447:VAL:HG23	1.93	0.52
1:B:59:ASN:HB3	1:B:208:MSE:CE	2.40	0.52
1:A:93:MSE:HG2	1:A:102:TRP:CZ2	2.45	0.51
1:B:422:PHE:HE2	1:B:436:MSE:CE	2.23	0.51
1:B:297:PHE:CE2	1:B:301:ILE:HD11	2.45	0.51
1:A:358:THR:C	1:A:360:GLY:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:PHE:HE1	1:A:446:CYS:CB	2.23	0.51
1:B:36:LEU:HA	1:B:152:ILE:HD11	1.91	0.51
1:B:145:PHE:O	1:B:149:MSE:HB2	2.11	0.51
1:A:333:LEU:HB2	1:A:351:VAL:HG11	1.93	0.51
1:B:78:LEU:HB3	1:B:136:LEU:HD13	1.91	0.51
1:B:38:ILE:HG21	1:B:228:ALA:HA	1.92	0.51
1:B:325:PHE:O	1:B:329:PHE:HD2	1.92	0.51
1:A:122:GLN:HG2	1:A:198:ASN:ND2	2.26	0.51
1:A:320:LEU:CD1	1:A:450:THR:HB	2.35	0.51
1:A:100:ARG:HG3	1:A:232:MSE:O	2.11	0.51
1:A:370:ILE:HD13	1:A:407:ILE:HG21	1.93	0.51
1:A:13:LEU:HB2	1:A:234:ASP:O	2.11	0.51
1:A:330:SER:OG	1:A:440:LEU:HA	2.10	0.51
1:B:100:ARG:CD	1:B:232:MSE:O	2.59	0.51
1:B:422:PHE:HE2	1:B:436:MSE:HE2	1.76	0.50
1:A:110:LEU:O	1:A:113:PRO:HD2	2.11	0.50
1:A:177:SER:HB2	1:A:296:PRO:HB2	1.92	0.50
1:A:83:GLY:O	1:A:87:ARG:HG3	2.11	0.50
1:B:51:MSE:HE2	1:B:273:ALA:HB2	1.94	0.50
1:B:65:PHE:HD1	1:B:67:PHE:CE2	2.29	0.50
1:B:432:PRO:HB2	1:B:436:MSE:CE	2.41	0.50
1:B:404:LEU:O	1:B:405:GLY:C	2.50	0.50
1:A:367:PHE:CZ	1:A:404:LEU:HG	2.48	0.49
1:B:186:VAL:HG21	1:B:216:ILE:HG13	1.95	0.49
1:B:78:LEU:N	1:B:78:LEU:HD13	2.28	0.49
1:A:265:PHE:CZ	2:A:501:NO3:O2	2.65	0.49
1:B:167:ILE:HG23	1:B:171:LEU:HD12	1.95	0.49
1:A:65:PHE:CE1	1:A:126:THR:HG23	2.45	0.49
1:A:366:THR:O	1:A:370:ILE:HD12	2.12	0.49
1:B:36:LEU:HA	1:B:152:ILE:CD1	2.43	0.49
1:A:71:GLN:HB3	1:A:128:PHE:CZ	2.48	0.49
1:A:418:ILE:O	1:A:419:PRO:C	2.50	0.48
1:A:174:LEU:O	1:A:178:VAL:HG12	2.13	0.48
1:B:75:LEU:O	1:B:79:PRO:HD3	2.13	0.48
1:B:52:LEU:H	1:B:179:MSE:HE2	1.78	0.48
1:A:175:GLY:HA2	1:A:178:VAL:HG12	1.96	0.48
1:A:260:LEU:O	1:A:263:ALA:HB3	2.14	0.48
1:A:269:ILE:HD11	1:A:415:GLY:H	1.79	0.48
1:A:302:ALA:O	1:A:361:LEU:HA	2.12	0.48
1:B:428:MSE:O	1:B:429:THR:HG22	2.13	0.48
1:A:52:LEU:HD23	1:A:179:MSE:CE	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:THR:O	1:A:363:SER:HB3	2.14	0.48
1:A:78:LEU:HD13	1:A:132:ILE:HG23	1.94	0.48
1:B:403:ALA:O	1:B:407:ILE:HG13	2.13	0.48
1:A:151:ASN:C	1:A:151:ASN:ND2	2.67	0.48
1:B:78:LEU:O	1:B:79:PRO:C	2.52	0.48
1:B:154:PHE:CB	1:B:235:ILE:HD11	2.44	0.48
1:A:358:THR:O	1:A:360:GLY:N	2.46	0.48
1:A:47:PHE:HE1	1:A:173:ASN:ND2	2.11	0.48
1:B:279:ALA:HB3	1:B:288:ILE:HD13	1.95	0.47
1:B:359:ALA:O	1:B:363:SER:HB2	2.14	0.47
1:B:264:THR:HB	1:B:363:SER:HA	1.95	0.47
1:B:36:LEU:HD12	1:B:152:ILE:HG12	1.96	0.47
1:A:171:LEU:HA	1:A:174:LEU:HB2	1.95	0.47
1:A:40:VAL:O	1:A:44:LEU:N	2.47	0.47
1:B:367:PHE:O	1:B:369:MSE:N	2.47	0.47
1:B:88:VAL:HG13	1:B:92:PHE:HE1	1.79	0.47
1:B:431:SER:OG	1:B:433:VAL:HG23	2.14	0.47
1:B:144:ASN:O	1:B:148:SER:HB3	2.15	0.47
1:A:27:LYS:O	1:A:30:HIS:N	2.46	0.47
1:A:324:ILE:HG13	1:A:324:ILE:H	1.59	0.47
1:B:53:PHE:CE2	1:B:135:ALA:HA	2.49	0.47
1:B:88:VAL:HB	1:B:89:PRO:HD3	1.96	0.47
1:A:342:SER:O	1:A:344:ASN:N	2.48	0.47
1:A:149:MSE:HE1	1:A:169:GLY:N	2.30	0.47
1:B:140:PHE:H	1:B:140:PHE:HD2	1.62	0.47
1:A:323:PHE:CD1	1:A:446:CYS:CB	2.92	0.47
1:B:153:SER:HB3	1:B:165:LEU:HD21	1.97	0.47
1:B:441:ILE:O	1:B:445:VAL:HG23	2.15	0.47
1:A:321:ILE:O	1:A:325:PHE:HD2	1.98	0.47
1:B:62:LYS:HB2	1:B:208:MSE:HE1	1.96	0.47
1:A:24:TRP:CZ3	1:A:157:PRO:HD3	2.50	0.46
1:A:264:THR:OG1	1:A:362:GLY:CA	2.64	0.46
1:B:82:SER:HB3	1:B:139:GLY:HA3	1.92	0.46
1:A:376:GLN:O	1:A:377:ILE:C	2.54	0.46
1:A:425:SER:OG	1:A:431:SER:O	2.33	0.46
1:A:379:ILE:CG2	1:A:380:TYR:N	2.78	0.46
1:A:271:PHE:O	1:A:275:PHE:CB	2.64	0.46
1:B:201:PRO:O	1:B:202:GLN:HG3	2.16	0.46
1:B:110:LEU:O	1:B:113:PRO:HD2	2.16	0.46
1:B:367:PHE:C	1:B:369:MSE:N	2.65	0.46
1:A:392:ALA:C	1:A:394:LYS:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:O	1:A:325:PHE:HB2	2.16	0.46
1:A:94:VAL:N	1:A:95:PRO:CD	2.78	0.46
1:A:78:LEU:CD1	1:A:132:ILE:HG23	2.45	0.45
1:B:43:LEU:HA	1:B:43:LEU:HD23	1.86	0.45
1:A:87:ARG:HG2	1:A:143:ALA:HA	1.98	0.45
1:A:420:GLN:HA	1:A:420:GLN:OE1	2.16	0.45
1:A:65:PHE:HE1	1:A:126:THR:CG2	2.29	0.45
1:B:189:VAL:O	1:B:212:ASN:ND2	2.50	0.45
1:A:125:ASN:HB2	1:B:123:ASN:OD1	2.17	0.45
1:A:403:ALA:O	1:A:407:ILE:HD12	2.16	0.45
1:B:265:PHE:O	1:B:268:PHE:HB3	2.16	0.45
1:B:295:GLY:HA3	1:B:356:PHE:CD2	2.52	0.45
1:A:61:ASN:HA	1:A:65:PHE:O	2.17	0.45
1:B:255:TRP:C	1:B:257:LEU:N	2.69	0.45
1:A:108:ALA:C	1:A:110:LEU:H	2.20	0.45
1:A:320:LEU:O	1:A:321:ILE:C	2.54	0.45
1:A:176:VAL:HG13	1:A:177:SER:H	1.81	0.45
1:B:437:LYS:O	1:B:441:ILE:HG12	2.17	0.45
1:A:22:ALA:O	1:A:23:PHE:C	2.56	0.45
1:A:362:GLY:O	1:A:366:THR:N	2.36	0.44
1:A:16:TRP:CD1	1:A:235:ILE:HD13	2.52	0.44
1:A:23:PHE:CD2	1:A:23:PHE:C	2.90	0.44
1:A:143:ALA:C	1:A:145:PHE:H	2.20	0.44
1:A:311:ASP:O	1:A:313:PHE:N	2.50	0.44
1:A:322:ASN:ND2	1:A:326:MSE:HE2	2.33	0.44
1:A:75:LEU:HG	1:A:128:PHE:HE2	1.83	0.44
1:A:325:PHE:O	1:A:328:ILE:HB	2.18	0.44
1:B:116:TRP:CH2	1:B:133:VAL:CG2	3.00	0.44
1:B:149:MSE:SE	1:B:168:ASN:HD22	2.51	0.44
1:A:228:ALA:O	1:A:232:MSE:HB2	2.18	0.44
1:A:275:PHE:O	1:A:278:LEU:N	2.51	0.44
1:B:136:LEU:O	1:B:139:GLY:N	2.50	0.44
1:B:130:ILE:HD13	1:B:130:ILE:HA	1.86	0.44
1:B:52:LEU:HA	1:B:179:MSE:SE	2.68	0.44
1:B:128:PHE:HE1	1:B:132:ILE:HD11	1.82	0.44
1:A:381:ARG:O	1:A:385:LYS:CB	2.66	0.44
1:B:339:GLY:C	1:B:341:GLY:H	2.21	0.44
1:B:342:SER:O	1:B:344:ASN:N	2.50	0.44
1:A:175:GLY:HA2	1:A:178:VAL:CG1	2.47	0.43
1:A:262:LEU:C	1:A:262:LEU:CD2	2.86	0.43
1:A:444:ILE:HG22	1:A:445:VAL:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:O	1:B:133:VAL:C	2.53	0.43
1:A:57:THR:HG21	1:A:72:LEU:O	2.18	0.43
1:A:179:MSE:HG3	1:A:180:GLN:N	2.33	0.43
1:B:129:GLY:HA2	1:B:132:ILE:HG13	2.00	0.43
1:B:271:PHE:CE2	1:B:418:ILE:HD13	2.53	0.43
1:A:151:ASN:HD22	1:A:151:ASN:C	2.20	0.43
1:B:293:PHE:O	1:B:294:PHE:C	2.56	0.43
1:B:67:PHE:CE1	1:B:128:PHE:CD2	3.01	0.43
1:A:262:LEU:O	1:A:262:LEU:HD23	2.18	0.43
1:A:34:ARG:HD2	1:A:231:GLY:O	2.18	0.43
1:B:78:LEU:O	1:B:81:VAL:N	2.47	0.43
1:A:24:TRP:CD1	1:A:29:LYS:HB3	2.53	0.43
1:A:379:ILE:HG23	1:A:380:TYR:N	2.34	0.43
1:A:270:GLY:HA3	1:A:418:ILE:HD12	2.00	0.43
1:B:288:ILE:O	1:B:292:ALA:N	2.51	0.43
1:B:116:TRP:CZ3	1:B:133:VAL:HG21	2.53	0.43
1:A:181:LEU:O	1:A:185:LEU:HG	2.19	0.43
1:A:203:ALA:C	1:A:205:GLY:H	2.21	0.43
1:B:83:GLY:O	1:B:85:LEU:N	2.51	0.43
1:B:48:CYS:SG	1:B:217:TRP:CZ3	3.04	0.43
1:B:116:TRP:CG	1:B:134:ILE:HD11	2.53	0.43
1:A:108:ALA:C	1:A:110:LEU:N	2.72	0.43
1:B:51:MSE:HB3	1:B:179:MSE:CE	2.49	0.42
1:B:323:PHE:HB3	1:B:447:VAL:CG2	2.48	0.42
1:B:45:LEU:HA	1:B:45:LEU:HD23	1.83	0.42
1:B:57:THR:HA	1:B:60:LEU:HD22	2.01	0.42
1:A:125:ASN:H	1:B:123:ASN:HD21	1.67	0.42
1:B:255:TRP:O	1:B:258:SER:N	2.52	0.42
1:B:116:TRP:CD1	1:B:134:ILE:HD11	2.55	0.42
1:A:429:THR:OG1	1:A:430:GLY:N	2.51	0.42
1:A:73:PHE:O	1:A:74:LEU:C	2.57	0.42
1:B:323:PHE:HE1	1:B:446:CYS:HB3	1.80	0.42
1:A:266:GLY:HA3	1:A:414:GLY:HA3	2.02	0.42
1:A:326:MSE:O	1:A:330:SER:HB2	2.20	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.64	0.42
1:B:268:PHE:HE2	1:B:299:GLY:HA3	1.85	0.42
1:A:303:ARG:HA	1:A:360:GLY:O	2.20	0.42
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.78	0.42
1:A:353:MSE:HE3	1:A:353:MSE:N	2.34	0.42
1:B:252:LEU:HA	1:B:255:TRP:HD1	1.85	0.42
1:B:67:PHE:HB2	1:B:72:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:H	1:B:335:LEU:CD1	2.33	0.42
1:A:160:LYS:HG2	1:A:160:LYS:H	1.60	0.42
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.72	0.42
1:B:140:PHE:C	1:B:142:GLY:H	2.23	0.42
1:B:101:ARG:O	1:B:104:VAL:HG12	2.20	0.42
1:A:267:SER:HB2	1:A:359:ALA:HB1	2.02	0.42
1:B:180:GLN:OE1	1:B:296:PRO:HG2	2.20	0.42
1:B:288:ILE:H	1:B:288:ILE:HG12	1.70	0.41
1:B:187:ILE:HG22	1:B:210:LEU:HA	2.02	0.41
1:A:337:LEU:HB3	1:A:338:PRO:HD2	2.02	0.41
1:B:255:TRP:O	1:B:257:LEU:N	2.53	0.41
1:A:47:PHE:CD1	1:A:173:ASN:HA	2.55	0.41
1:A:264:THR:HG21	1:A:366:THR:OG1	2.20	0.41
1:B:109:ILE:HG13	1:B:109:ILE:H	1.53	0.41
1:B:64:GLY:O	1:B:124:PRO:HB3	2.21	0.41
1:A:113:PRO:HB3	1:A:137:LEU:HB3	2.01	0.41
1:B:112:ILE:O	1:B:113:PRO:C	2.57	0.41
1:A:79:PRO:HD3	1:A:135:ALA:HB1	2.01	0.41
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.80	0.41
1:B:171:LEU:O	1:B:174:LEU:HB2	2.21	0.41
1:A:16:TRP:NE1	1:A:154:PHE:O	2.53	0.41
1:A:156:PHE:HD1	1:A:160:LYS:HG3	1.85	0.41
1:B:216:ILE:HD13	1:B:216:ILE:HA	1.92	0.41
1:A:318:VAL:O	1:A:321:ILE:HG23	2.21	0.41
1:B:222:ALA:O	1:B:225:THR:HG22	2.20	0.41
1:B:57:THR:HA	1:B:60:LEU:HB2	2.02	0.41
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.79	0.41
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.94	0.41
1:B:93:MSE:CG	1:B:102:TRP:CZ3	3.02	0.41
1:B:255:TRP:O	1:B:256:LEU:C	2.58	0.41
1:A:100:ARG:O	1:A:101:ARG:C	2.59	0.41
1:B:310:SER:HB2	1:B:315:GLY:HA2	2.03	0.41
1:A:39:SER:OG	1:A:148:SER:OG	2.39	0.41
1:A:40:VAL:CG2	1:A:41:SER:N	2.84	0.41
1:B:45:LEU:HD11	1:B:220:LEU:HB3	2.02	0.41
1:A:428:MSE:HG3	1:A:428:MSE:H	1.69	0.41
1:B:126:THR:HG22	1:B:131:PHE:CE2	2.55	0.40
1:A:93:MSE:HG2	1:A:102:TRP:CZ3	2.55	0.40
1:A:59:ASN:HB3	1:A:208:MSE:HE3	2.02	0.40
1:A:376:GLN:HA	1:A:379:ILE:HG22	2.02	0.40
1:B:333:LEU:O	1:B:336:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLN:HG3	1:B:338:PRO:CG	2.51	0.40
1:B:12:LEU:CD2	1:B:13:LEU:N	2.71	0.40
1:B:262:LEU:HG	1:B:410:ILE:O	2.21	0.40
1:A:269:ILE:HA	1:A:272:SER:HB2	2.03	0.40
1:B:77:ALA:O	1:B:416:PHE:HA	2.20	0.40
1:B:345:PHE:O	1:B:348:PHE:HB3	2.20	0.40
1:A:265:PHE:O	1:A:268:PHE:N	2.55	0.40
1:B:171:LEU:HD23	1:B:174:LEU:HD12	2.04	0.40
1:A:410:ILE:HA	1:A:410:ILE:HD12	1.87	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	416/468 (89%)	308 (74%)	83 (20%)	25 (6%)	2	11
1	B	421/468 (90%)	327 (78%)	75 (18%)	19 (4%)	3	18
All	All	837/936 (89%)	635 (76%)	158 (19%)	44 (5%)	2	15

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	231	GLY
1	A	305	VAL
1	A	312	LYS
1	A	432	PRO
1	B	52	LEU
1	B	54	SER
1	B	230	SER
1	B	291	LEU

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	343	GLY
1	A	380	TYR
1	A	444	ILE
1	B	83	GLY
1	B	194	PHE
1	B	315	GLY
1	B	332	LEU
1	B	368	GLN
1	B	453	VAL
1	A	204	ASP
1	A	304	SER
1	A	421	ALA
1	B	164	ALA
1	B	232	MSE
1	A	27	LYS
1	A	87	ARG
1	A	144	ASN
1	A	311	ASP
1	A	430	GLY
1	B	26	ASN
1	B	51	MSE
1	B	231	GLY
1	A	53	PHE
1	A	332	LEU
1	B	84	ALA
1	B	376	GLN
1	A	88	VAL
1	A	169	GLY
1	A	325	PHE
1	A	377	ILE
1	A	157	PRO
1	A	433	VAL
1	B	127	PRO
1	B	343	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	299/356 (84%)	246 (82%)	53 (18%)	2	10
1	B	304/356 (85%)	246 (81%)	58 (19%)	2	8
All	All	603/712 (85%)	492 (82%)	111 (18%)	2	9

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	37	TRP
1	A	43	LEU
1	A	57	THR
1	A	66	ASN
1	A	68	THR
1	A	69	THR
1	A	70	ASP
1	A	72	LEU
1	A	76	THR
1	A	91	SER
1	A	93	MSE
1	A	110	LEU
1	A	112	ILE
1	A	114	CYS
1	A	126	THR
1	A	149	MSE
1	A	151	ASN
1	A	160	LYS
1	A	163	SER
1	A	174	LEU
1	A	177	SER
1	A	189	VAL
1	A	191	VAL
1	A	195	LEU
1	A	204	ASP
1	A	208	MSE
1	A	221	LEU
1	A	233	ASN
1	A	234	ASP
1	A	269	ILE
1	A	277	MSE
1	A	280	LYS

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Mol	Chain	Res	Type
1	A	285	ASP
1	A	286	VAL
1	A	298	ILE
1	A	316	VAL
1	A	319	THR
1	A	320	LEU
1	A	321	ILE
1	A	324	ILE
1	A	332	LEU
1	A	352	PHE
1	A	353	MSE
1	A	370	ILE
1	A	406	PHE
1	A	410	ILE
1	A	413	VAL
1	A	431	SER
1	A	436	MSE
1	A	448	LEU
1	A	451	TRP
1	B	15	ASP
1	B	20	ASN
1	B	35	ASN
1	B	40	VAL
1	B	43	LEU
1	B	51	MSE
1	B	56	VAL
1	B	70	ASP
1	B	74	LEU
1	B	78	LEU
1	B	82	SER
1	B	85	LEU
1	B	93	MSE
1	B	105	PHE
1	B	121	VAL
1	B	126	THR
1	B	133	VAL
1	B	136	LEU
1	B	151	ASN
1	B	160	LYS
1	B	163	SER
1	B	176	VAL
1	B	185	LEU

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Mol	Chain	Res	Type
1	B	202	GLN
1	B	204	ASP
1	B	206	SER
1	B	210	LEU
1	B	216	ILE
1	B	235	ILE
1	B	257	LEU
1	B	259	LEU
1	B	262	LEU
1	B	264	THR
1	B	267	SER
1	B	277	MSE
1	B	288	ILE
1	B	289	LEU
1	B	291	LEU
1	B	309	ILE
1	B	318	VAL
1	B	320	LEU
1	B	332	LEU
1	B	333	LEU
1	B	336	THR
1	B	340	THR
1	B	352	PHE
1	B	367	PHE
1	B	368	GLN
1	B	373	ILE
1	B	406	PHE
1	B	413	VAL
1	B	416	PHE
1	B	425	SER
1	B	427	ASN
1	B	429	THR
1	B	436	MSE
1	B	440	LEU
1	B	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	122	GLN
1	A	168	ASN

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	287	ASN
1	B	173	ASN
1	B	420	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](#)

1 ligand is 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	NO3	A	501	-	3,3,3	2.64	2 (66%)	3,3,3	0.48	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	NO3	A	501	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NO3	O2-N	3.18	1.41	1.25
2	A	501	NO3	O3-N	3.25	1.42	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NO3	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	408/468 (87%)	-0.25	11 (2%) 58 35	18, 43, 91, 145	0
1	B	414/468 (88%)	-0.16	17 (4%) 41 19	16, 33, 96, 141	0
All	All	822/936 (87%)	-0.21	28 (3%) 49 25	16, 37, 94, 145	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	THR	4.9
1	B	393	HIS	4.6
1	B	244	ASP	4.5
1	A	12	LEU	4.5
1	B	12	LEU	4.0
1	B	392	ALA	3.8
1	B	380	TYR	3.8
1	A	340	THR	3.6
1	B	313	PHE	3.6
1	A	13	LEU	3.5
1	B	204	ASP	3.5
1	A	14	ARG	3.5
1	B	13	LEU	3.3
1	B	314	GLY	3.2
1	B	243	ALA	3.0
1	A	345	PHE	2.9
1	B	205	GLY	2.7
1	B	381	ARG	2.7
1	A	15	ASP	2.7
1	A	317	ARG	2.6
1	A	452	LEU	2.6
1	A	379	ILE	2.6
1	B	372	VAL	2.5
1	B	395	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	335	LEU	2.5
1	B	374	PHE	2.4
1	A	308	ALA	2.1
1	B	377	ILE	2.1

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
2	NO3	A	501	4/4	0.85	0.85	12.90	64,68,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.